MedeA QSPR

Contents

1 Key Benefits of *MedeA QSPR*

- Determination of geometric descriptors for organic molecules
- Evaluation of thermodynamic properties (of organic compounds) based on Group contributions
- Rapid property calculation enabling screening of compounds and/or providing input conditions for molecular simulations
- Provides thermophysical properties (based on Joback's Group Contribution method)
- Uses group contributions to compute properties based on correlations

2 Introduction

"*MedeA QSPR*: Property Prediction using Group Contributions" employs correlations to predict thermophysical properties, based on the chemical groups that constitute an organic molecule. The number and type of groups, and their contribution to each property, have been developed and described by Joback and Reid [1]. Only structural information of a chemical compound (a molecule) is used to calculate thermophysical and transport properties, by adding group parameters. This method uses a single group list for all eleven properties, therefore, allowing the calculation of all properties from a single analysis.

3 Molecular Descriptors

There are 42 molecular descriptors (i.e. groups) in the Joback & Reid method [1]. These molecular descriptors are listed below, along with a short description and the name of the "*MedeA* variable" that is associated with each descriptor. *MedeA* variables are useful when printing these quantities in user-defined tables, as part of a flowchart involving a QSPR stage.

[1] Kevin G Joback and Robert C Reid, "Estimation of Pure-Component Properties From Group-Contributions," *Chemical Engineering Communications* 57, no. 1 (February 5, 1987): 233-243.

Table1: Descriptors, *MedeA* variables and a summary of each descriptor.

Descriptor	*MedeA* variable	Description
NC0	qspr_NC0_calc	-C atoms with zero contribution, member of another group
NC1	qspr_NC1_calc	-CH_3 groups, non-ring
NC2	qspr_NC2_calc	-CH_2 groups, non-ring
NC3	qspr_NC3_calc	-CH groups, non-ring
NC4	qspr_NC4_calc	-C atoms, non-ring
NC5	qspr_NC5_calc	=CH_2 groups, non-ring
NC6	qspr_NC6_calc	=CH groups, non-ring
NC7	qspr_NC7_calc	=C atoms, non-ring
NC8	qspr_NC8_calc	=C= atoms, non-ring
NC9	qspr_NC9_calc	#CH groups, non-ring
NC10	qspr_NC10_calc	#C atoms, non-ring
NC11	qspr_NC11_calc	-CH_2 non-aromatic groups, ring
NC12	qspr_NC12_calc	-CH non-aromatic groups, ring
NC13	qspr_NC13_calc	-C non-aromatic atoms, ring
NC14	qspr_NC14_calc	=CH aromatic groups, ring
NC15	qspr_NC15_calc	=C aromatic atoms, ring
NF1	qspr_NF1_calc	F atoms
NCl1	qspr_NCl1_calc	Cl atoms
NBr1	qspr_NBr1_calc	Br atoms
NI1	qspr_NI1_calc	I atoms
NO1	qspr_NO1_calc	-O- groups in OH, in alcohols
NO2	qspr_NO2_calc	-O- groups in OH, in phenol
NO3	qspr_NO3_calc	-O- groups in ethers, non-ring
NO4	qspr_NO4_calc	-O- groups in ethers, ring
NO5	qspr_NO5_calc	=O groups, non-ring
NO6	qspr_NO6_calc	=O groups, ring
NO7	qspr_NO7_calc	=O groups in aldehydes
NO8	qspr_NO8_calc	-O- groups in carboxylic acid groups
NO9	qspr_NO9_calc	-O- groups in carboxylic ester groups
NO10	qspr_NO10_calc	=O groups in other than NO1-NO9 groups
NN1	qspr_NN1_calc	-NH_2 groups, in primary amines
NN2	qspr_NN2_calc	-NH groups, in secondary amines, non-ring
NN3	qspr_NN3_calc	-NH groups, in secondary amines, ring
NN4	qspr_NN4_calc	-N atoms in tertiary amines, non-ring
NN5	qspr_NN5_calc	-N= atoms, nonring
NN6	qspr_NN6_calc	-N= atoms, ring
NN7	qspr_NN7_calc	=NH groups
NN8	qspr_NN8_calc	CN- groups, in cyanides
NN9	qspr_NN9_calc	-NO_2 groups
NS1	qspr_NS1_calc	-SH groups, in thiols
NS2	qspr_NS2_calc	-S atoms, non-ring
NS3	qspr_NS3_calc	-S- atoms, ring
NH1	qspr_NH1_calc	-H atoms with zero contribution, member of another group

4 Properties

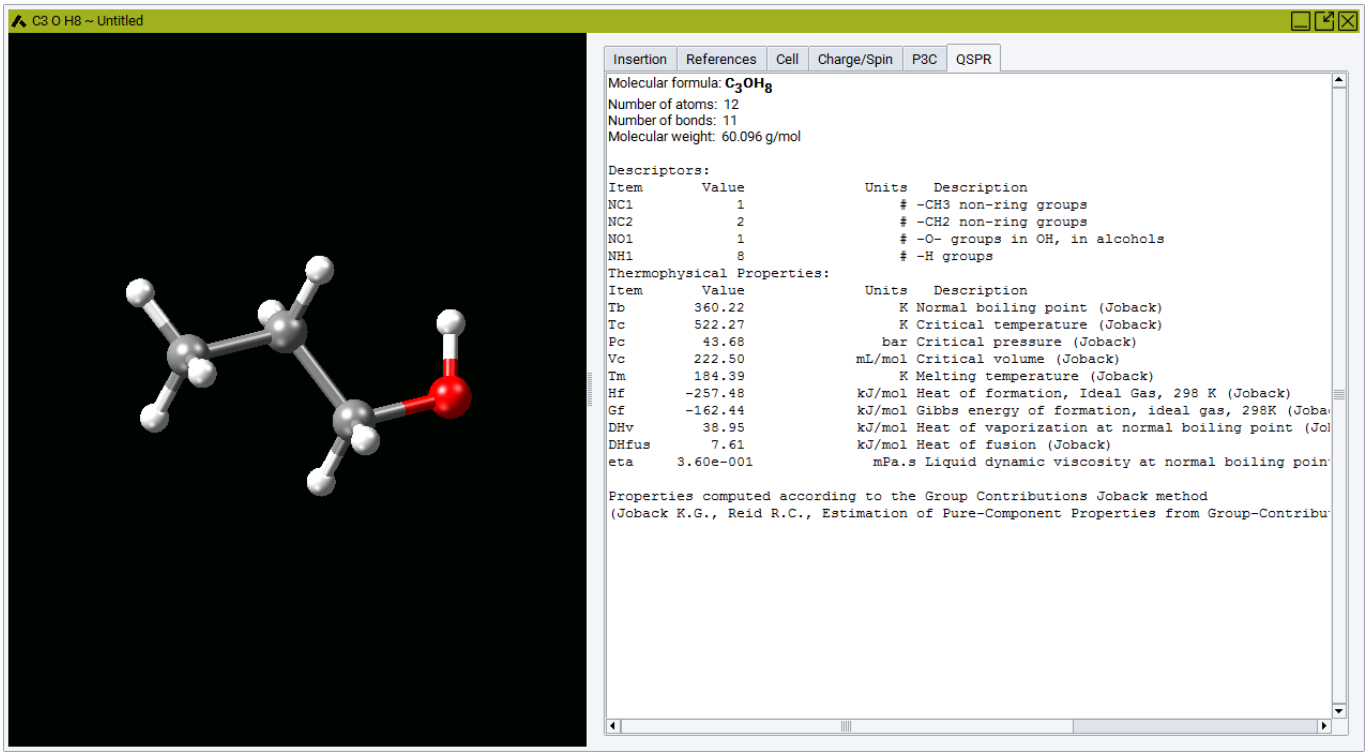
There are ten properties calculated using the Joback & Reid method [1].

Table2: Properties, *MedeA* variables and a description of each property.

Property	Units	*MedeA* variable	Description
Tb	K	qspr_Tb_calc	Normal Boiling Point Temperature
Tc	K	qspr_Tc_calc	Critical Temperature
Pc	bar	qspr_Pc_calc	Critical Pressure
Vc	ml/mol	qspr_Vc_calc	Critical Volume
Tm	K	qspr_Tm_calc	Melting Temperature
Hf	kJ/mol	qspr_Hf_calc	Heat of Formation, ideal gas, 298 K
Gf	kJ/mol	qspr_Gf_calc	Gibbs Energy of Formation, ideal gas, 298 K
DHv	kJ/mol	qspr_DHv_calc	Heat of Vaporization at normal boiling point
DHfus	kJ/mol	qspr_DHfus_calc.	Heat of Fusion
Eta	mPas	qspr_eta_calc	Liquid Dynamic Viscosity at normal boiling point

Both the molecular descriptors and the calculated properties are available interactively in the *Molecular Builder*, or through a QSPR: Property Prediction using Group Contributions stage in a *MedeA* flowchart.

The results for propanol appear as shown here on the *QSPR* tab of the *Molecular Builder* and the output of a QSPR: Property Prediction using Group Contributions stage looks like this in *Job.out*.



DOCUMENTATION

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Stage 1: Property Prediction using Group Contributions

Molecular formula: C3OH8
Number of atoms:  12
Number of bonds:  11
Molecular weight:  60.096 g/mol

Descriptors:
Item       Value              Units   Description
NC1            1                  # -CH3 non-ring groups
NC2            2                  # -CH2 non-ring groups
NO1            1                  # -O- groups in OH, in alcohols
NH1            8                  # -H groups
Thermophysical Properties:
Item       Value              Units   Description
Tb        360.22                  K Normal boiling point (Joback)
Tc        522.27                  K Critical temperature (Joback)
Pc         43.68                bar Critical pressure (Joback)
Vc        222.50             mL/mol Critical volume (Joback)
Tm        184.39                  K Melting temperature (Joback)
Hf       -257.48             kJ/mol Heat of formation, Ideal Gas, 298 K (Joback)
Gf       -162.44             kJ/mol Gibbs energy of formation, ideal gas, 298K (Joback)
DHv        38.95             kJ/mol Heat of vaporization at normal boiling point (Joback)
DHfus       7.61             kJ/mol Heat of fusion (Joback)
eta     3.60e-001               mPa.s Liquid dynamic viscosity at normal boiling point (Joback)

Properties computed according to the Group Contributions Joback method
(Joback K.G., Reid R.C., Estimation of Pure-Component Properties from Group-Contributions, Chem. Eng. Commun. 57, p. 233-243 (1987)


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