azadirachtin

Inchi: InChI=1S/C35H44O16/c1-8-15(2)24(38)49-18-12-19(48-16(3)36)32(26(39)43-6)13-46-21
InchiKey: FTNJWQUOZFUQQJ-UHFFFAOYSA-N
Formula: C35H44O16
SMILES: CC=C(C)C(=O)OC1CC(OC(C)=O)C2(C(=O)OC)COC3C2C12COC(O)(C(=O)OC)C2C(C)
Mol. weight [g/mol]: 720.72

Physical Properties

Property code	Value	Unit	Source
gf	-1081.70	kJ/mol	Joback Method
hf	-2188.53	kJ/mol	Joback Method
hfus	93.09	kJ/mol	Joback Method
hvap	192.34	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	-0.203		Crippen Method
mcvol	485.250	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
tb	1750.90	K	Joback Method
tc	2466.26	K	Joback Method
tf	447.15 ± 1.00	K	Solubility of Azadirachtin in Supercritical Carbon Dioxide at Several Temperatures
vc	1.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	5302.78	J/mol×K	1750.90	Joback Method
cpg	6504.17	J/mol×K	1870.13	Joback Method
cpg	7963.96	J/mol×K	1989.35	Joback Method
cpg	9710.15	J/mol×K	2108.58	Joback Method
cpg	11770.75	J/mol×K	2227.80	Joback Method
cpg	14173.78	J/mol×K	2347.03	Joback Method
cpg	16947.24	J/mol×K	2466.26	Joback Method

Sources

Solubility of Azadirachtin in Supercritical Carbon Dioxide at Several Temperatures:	https://www.doi.org/10.1021/je200239p
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume