Andrographolide

Other names:	(S,E)-4-hydroxy-3-(2-((1R,4aS,5R,6R,8aS)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2- 2(3H)-Furanone, 3-[2-[decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl] 3-[2-[decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylenenaphthyl]ethylid
Inchi:	InChI=1S/C20H30O5/c1-12-4-7-16-19(2,9-8-17(23)20(16,3)11-21)14(12)6-5-13-15(22)10
InchiKey:	BOJKULTULYSRAS-ACAGNQJTSA-N
Formula:	C20H30O5
SMILES:	C=C1CCC2C(C)(CO)C(O)CCC2(C)C1CC=C1C(=O)OCC1O
Mol. weight [g/mol]:	350.45
CAS:	5508-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-327.57	kJ/mol	Joback Method
hf	-871.35	kJ/mol	Joback Method
hfus	38.89	kJ/mol	Joback Method
hvap	117.40	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	1.963		Crippen Method
mcvol	276.530	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
ripol	2635.00		NIST Webbook
ripol	2635.00		NIST Webbook
tb	1066.42	K	Joback Method
tc	1305.62	K	Joback Method
tf	684.23	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.71	J/mol×K	1066.42	Joback Method
cpg	1114.87	J/mol×K	1106.29	Joback Method
cpg	1143.26	J/mol×K	1146.15	Joback Method
cpg	1173.17	J/mol×K	1186.02	Joback Method

cpg	1204.88	J/mol×K	1225.89	Joback Method
cpg	1238.66	J/mol×K	1265.76	Joback Method
cpg	1274.79	J/mol×K	1305.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5508587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Andrographolide in Various Solvents from (288.2 to 323.2) K:	https://www.doi.org/10.1021/je100344z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume