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)C1C/C=C1\C(=O)OCC1O

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
hfus	38.89	kJ/mol	Joback Method
logp	1.963		Crippen Method
mcvol	276.530	ml/mol	McGowan Method
ripol	2635.00		NIST Webbook
ripol	2635.00		NIST Webbook

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility of Andrographolide in Various Solvents from (288.2 to 323.2) K:	https://www.doi.org/10.1021/je100344z
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5508587&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices