Hanphyllin

Inchi: InChI=1S/C15H20O3/c1-9-4-6-12-11(3)15(17)18-14(12)8-10(2)13(16)7-5-9/h5,8,12-14,1
InchiKey: XQVSREKNQZKAKU-MUDDOMJDSA-N
Formula: C15H20O3
SMILES: C=C1C(=O)OC2C=C(C)C(O)CC=C(C)CCC12
Mol. weight [g/mol]: 248.32
CAS: 60268-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-147.28	kJ/mol	Joback Method
hf	-515.86	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	77.21	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.522		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	775.69	K	Joback Method
tc	1001.07	K	Joback Method
tf	461.66	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.65	J/mol×K	775.69	Joback Method
cpg	644.79	J/mol×K	813.25	Joback Method
cpg	660.50	J/mol×K	850.82	Joback Method
cpg	674.78	J/mol×K	888.38	Joback Method
cpg	687.59	J/mol×K	925.94	Joback Method
cpg	698.93	J/mol×K	963.50	Joback Method
cpg	708.77	J/mol×K	1001.07	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60268408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume