Dihydroqinghaosu

Other names: DIHYDROARTEMISININ
Inchi: InChI=1S/C15H24O5/c1-8-4-5-11-9(2)12(16)17-13-15(11)10(8)6-7-14(3,18-13)19-20-15/
InchiKey: BJDCWCLMFKKGEE-UHFFFAOYSA-N
Formula: C15H24O5
SMILES: CC1CCC2C(C)C(O)OC3OC4(C)CCC1C32OO4
Mol. weight [g/mol]: 284.35

Physical Properties

Property code	Value	Unit	Source
gf	-253.10	kJ/mol	Joback Method
hf	-817.48	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.187		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1964.00		NIST Webbook
tb	768.42	K	Joback Method
tc	991.95	K	Joback Method
tf	514.43	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.74	J/mol×K	768.42	Joback Method
cpg	750.96	J/mol×K	805.67	Joback Method
cpg	770.85	J/mol×K	842.93	Joback Method
cpg	790.67	J/mol×K	880.18	Joback Method
cpg	810.71	J/mol×K	917.44	Joback Method
cpg	831.25	J/mol×K	954.69	Joback Method
cpg	852.57	J/mol×K	991.95	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=U126038&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