Deoxyartemisinin

Inchi: InChI=1S/C15H22O4/c1-8-4-5-11-9(2)12(16)17-13-15(11)10(8)6-7-14(3,18-13)19-15/h8-
InchiKey: ZQGMLVQZBIKKMP-UHFFFAOYSA-N
Formula: C15H22O4
SMILES: CC1CCC2C(C)C(=O)OC3OC4(C)CCC1C32O4
Mol. weight [g/mol]: 266.33
CAS: 72826-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-132.94	kJ/mol	Joback Method
hf	-644.45	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	63.70	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.463		Crippen Method
mcvol	197.950	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	2058.40		NIST Webbook
rinpol	2058.40		NIST Webbook
tb	717.51	K	Joback Method
tc	966.63	K	Joback Method
tf	503.02	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.96	J/mol×K	717.51	Joback Method
cpg	681.62	J/mol×K	759.03	Joback Method
cpg	703.54	J/mol×K	800.55	Joback Method
cpg	725.06	J/mol×K	842.07	Joback Method
cpg	746.56	J/mol×K	883.59	Joback Method
cpg	768.40	J/mol×K	925.11	Joback Method
cpg	790.94	J/mol×K	966.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C72826632&Units=SI

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