Dihydroartemisinin, 3-desoxy-

Other names: Deoxydihydroqinghaosu
Inchi: InChI=1S/C15H24O4/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: JQGOBHOUYKYFPD-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: CC1CCC2C(C)C(O)OC3OC4(C)CCC1C32O4
Mol. weight [g/mol]: 268.35
CAS: 72807-92-2

Physical Properties

Property code	Value	Unit	Source
gf	-154.88	kJ/mol	Joback Method
hf	-679.32	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	75.82	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.255		Crippen Method
mcvol	202.250	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	737.20	K	Joback Method
tc	956.73	K	Joback Method
tf	491.38	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.11	J/mol×K	737.20	Joback Method
cpg	713.02	J/mol×K	773.79	Joback Method
cpg	732.44	J/mol×K	810.38	Joback Method
cpg	751.66	J/mol×K	846.97	Joback Method
cpg	770.95	J/mol×K	883.56	Joback Method
cpg	790.60	J/mol×K	920.14	Joback Method
cpg	810.86	J/mol×K	956.73	Joback Method

Sources

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=C72807922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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