

8-epi-1,2-Dihydroartemisin

Inchi:	InChI=1S/C16H22O3/c1-8-7-16(4)6-5-11(17)9(2)13(16)14-12(8)10(3)15(18)19-14/h8,10,
InchiKey:	WTVNWPMSXICFCN-XGTCKSAYSA-N
Formula:	C16H22O3
SMILES:	CC1=C2C3OC(=O)C(C)C3C(C)CC2(C)CCC1=O
Mol. weight [g/mol]:	262.34

Physical Properties

Property code	Value	Unit	Source
gf	-123.82	kJ/mol	Joback Method
hf	-577.81	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	64.49	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.890		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	2107.00		NIST Webbook
tb	765.39	K	Joback Method
tc	1013.29	K	Joback Method
tf	514.05	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.67	J/mol×K	765.39	Joback Method
cpg	701.67	J/mol×K	806.71	Joback Method
cpg	722.58	J/mol×K	848.02	Joback Method
cpg	742.51	J/mol×K	889.34	Joback Method
cpg	761.61	J/mol×K	930.66	Joback Method
cpg	780.01	J/mol×K	971.97	Joback Method
cpg	797.84	J/mol×K	1013.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R419242&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

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