

Dihydroartemisinic aldehyde

Inchi:	InChI=1S/C15H24O/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)15(13)8-10/h8-9,11-15H,4-7H2
InchiKey:	PIUSZJFEZXYOAT-OKMQTDMMSA-N
Formula:	C15H24O
SMILES:	CC1=CC2C(C(C)C=O)CCC(C)C2CC1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	51.47	kJ/mol	Joback Method
hf	-317.20	kJ/mol	Joback Method
hfus	24.22	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.840		Crippen Method
mvol	197.760	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	616.18	K	Joback Method
tc	831.10	K	Joback Method
tf	312.41	K	Joback Method
vc	0.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.04	J/mol×K	616.18	Joback Method
cpg	652.72	J/mol×K	795.28	Joback Method
cpg	635.50	J/mol×K	759.46	Joback Method
cpg	617.07	J/mol×K	723.64	Joback Method
cpg	597.38	J/mol×K	687.82	Joback Method
cpg	576.39	J/mol×K	652.00	Joback Method
cpg	668.77	J/mol×K	831.10	Joback Method
dvisc	0.0004859	Paxs	616.18	Joback Method

dvisc	0.0005728	Paxs	565.55	Joback Method
dvisc	0.0006975	Paxs	514.92	Joback Method
dvisc	0.0008866	Paxs	464.30	Joback Method
dvisc	0.0011950	Paxs	413.67	Joback Method
dvisc	0.0017507	Paxs	363.04	Joback Method
dvisc	0.0029027	Paxs	312.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R603828&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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