Dihydroartemisinic aldehyde, isomer # 1

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
mcvol	197.760	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
ripol	2096.00		NIST Webbook
ripol	2096.00		NIST Webbook
tb	616.18	K	Joback Method
tc	831.10	K	Joback Method
tf	312.41	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.04	J/mol×K	616.18	Joback Method
cpg	576.39	J/mol×K	652.00	Joback Method
cpg	597.38	J/mol×K	687.82	Joback Method
cpg	617.07	J/mol×K	723.64	Joback Method
cpg	635.50	J/mol×K	759.46	Joback Method
cpg	652.72	J/mol×K	795.28	Joback Method
cpg	668.77	J/mol×K	831.10	Joback Method
dvisc	0.0029027	Pa×s	312.41	Joback Method

dvisc	0.0017507	Pa×s	363.04	Joback Method
dvisc	0.0011950	Pa×s	413.67	Joback Method
dvisc	0.0008866	Pa×s	464.30	Joback Method
dvisc	0.0006975	Pa×s	514.92	Joback Method
dvisc	0.0005728	Pa×s	565.55	Joback Method
dvisc	0.0004859	Pa×s	616.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603833&Units=SI
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

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