

Dihydroartemisinic acid

Inchi:	InChI=1S/C15H24O2/c1-9-4-6-12-10(2)5-7-13(14(12)8-9)11(3)15(16)17/h8,10-14H,4-7H
InchiKey:	JYGAZEJXUVDYHI-DDMQOUJLSA-N
Formula:	C15H24O2
SMILES:	CC1=CC2C(CC1)C(C)CCC2C(C)C(=O)O
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-114.75	kJ/mol	Joback Method
hf	-496.43	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	72.87	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.726		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
ripol	3016.00		NIST Webbook
tb	713.57	K	Joback Method
tc	918.78	K	Joback Method
tf	381.16	K	Joback Method
vc	0.760	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.91	J/molxK	713.57	Joback Method
cpg	645.17	J/molxK	747.77	Joback Method
cpg	662.28	J/molxK	781.97	Joback Method
cpg	678.28	J/molxK	816.18	Joback Method
cpg	693.21	J/molxK	850.38	Joback Method
cpg	707.11	J/molxK	884.58	Joback Method
cpg	720.03	J/molxK	918.78	Joback Method
dvisc	0.0042197	Paxs	381.16	Joback Method
dvisc	0.0016037	Paxs	436.56	Joback Method

dvisc	0.0007578	Paxs	491.96	Joback Method
dvisc	0.0004168	Paxs	547.37	Joback Method
dvisc	0.0002559	Paxs	602.77	Joback Method
dvisc	0.0001705	Paxs	658.17	Joback Method
dvisc	0.0001210	Paxs	713.57	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=R603813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	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

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