Artemisinic acid

Inchi: InChI=1S/C15H22O2/c1-9-4-6-12-10(2)5-7-13(14(12)8-9)11(3)15(16)17/h8,10,12-14H,3-
InchiKey: PLQMEXSCSAIXGB-SAXRGWBVSA-N
Formula: C15H22O2
SMILES: C=C(C(=O)O)C1CCC(C)C2CCC(C)=CC12
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-33.02	kJ/mol	Joback Method
hf	-375.51	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	72.67	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.646		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
ripol	3151.00		NIST Webbook
tb	710.57	K	Joback Method
tc	918.54	K	Joback Method
tf	380.44	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.72	J/mol×K	710.57	Joback Method
cpg	619.40	J/mol×K	745.23	Joback Method
cpg	635.94	J/mol×K	779.89	Joback Method
cpg	651.40	J/mol×K	814.56	Joback Method
cpg	665.82	J/mol×K	849.22	Joback Method
cpg	679.25	J/mol×K	883.88	Joback Method
cpg	691.75	J/mol×K	918.54	Joback Method

Sources

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=R603808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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