Dehydrogeosinin

Inchi: InChI=1S/C12H20O/c1-9-5-3-7-12(2)8-4-6-10(13)11(9)12/h4,6,9-11,13H,3,5,7-8H2,1-2H
InchiKey: KFMOLQKUBDSAST-MBYGNEARSA-N
Formula: C12H20O
SMILES: CC1CCCC2(C)CC=CC(O)C12
Mol. weight [g/mol]: 180.29

Physical Properties

Property code	Value	Unit	Source
gf	-4.51	kJ/mol	Joback Method
hf	-289.94	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.750		Crippen Method
mcvol	159.790	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
tb	586.76	K	Joback Method
tc	796.45	K	Joback Method
tf	323.80	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.54	J/mol×K	586.76	Joback Method
cpg	456.27	J/mol×K	621.71	Joback Method
cpg	473.88	J/mol×K	656.66	Joback Method
cpg	490.51	J/mol×K	691.61	Joback Method
cpg	506.27	J/mol×K	726.55	Joback Method
cpg	521.27	J/mol×K	761.50	Joback Method
cpg	535.65	J/mol×K	796.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R626514&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

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