15-Hydroxydehydroabietic acid, methyl ester

Other names: Methyl 15-hydroxydehydroabietate
Inchi: InChI=1S/C21H30O3/c1-19(2,23)15-8-9-16-14(13-15)7-10-17-20(16,3)11-6-12-21(17,4)1
InchiKey: IGUDTNVZIOWVIV-UHFFFAOYSA-N
Formula: C21H30O3
SMILES: COC(=O)C1(C)CCCC2(C)c3ccc(C(C)(C)O)cc3CCC12
Mol. weight [g/mol]: 330.46
CAS: 29461-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-70.20	kJ/mol	Joback Method
hf	-525.54	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.097		Crippen Method
mcvol	274.580	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2521.00		NIST Webbook
tb	899.59	K	Joback Method
tc	1127.76	K	Joback Method
tf	585.69	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.19	J/mol×K	899.59	Joback Method
cpg	951.75	J/mol×K	937.62	Joback Method
cpg	974.89	J/mol×K	975.65	Joback Method
cpg	998.89	J/mol×K	1013.67	Joback Method
cpg	1024.08	J/mol×K	1051.70	Joback Method
cpg	1050.77	J/mol×K	1089.73	Joback Method
cpg	1079.26	J/mol×K	1127.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29461232&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
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