13Alpha-delta(8)-dihydroabietic acid

Other names: Abietic acid, 13«alpha»H-«delta»8-dihydro-
Inchi: InChI=1S/C20H32O2/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(16,3)10-5-11-20(17,4)18(21
InchiKey: OEILFLGOGZTONZ-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CC(C)C1CCC2=C(CCC3C(C)(C(=O)O)CCCC23C)C1
Mol. weight [g/mol]: 304.47
CAS: 17611-16-4

Physical Properties

Property code	Value	Unit	Source
gf	-36.90	kJ/mol	Joback Method
hf	-493.64	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.430		Crippen Method
mcvol	263.220	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2491.90		NIST Webbook
rinpol	2491.90		NIST Webbook
tb	849.11	K	Joback Method
tc	1071.56	K	Joback Method
tf	516.49	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.94	J/mol×K	849.11	Joback Method
cpg	919.80	J/mol×K	886.18	Joback Method
cpg	942.70	J/mol×K	923.26	Joback Method
cpg	965.91	J/mol×K	960.33	Joback Method
cpg	989.73	J/mol×K	997.41	Joback Method
cpg	1014.40	J/mol×K	1034.48	Joback Method

cpg	1040.22	J/mol×K	1071.56	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=C17611164&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume