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

Physical Properties

Property code	Value	Unit	Source
hfus	22.54	kJ/mol	Joback Method
logp	5.430		Crippen Method
mcvol	263.220	ml/mol	McGowan Method
rinpol	2491.90		NIST Webbook
rinpol	2491.90		NIST Webbook

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17611164&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices