

Epidehydroabietol

Other names:	4-epi-Dehydroabietol
Inchi:	InChI=1S/C20H30O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/
InchiKey:	WSKGRAGZAQRSED-YPJRHXLCSA-N
Formula:	C20H30O
SMILES:	<chem>CC(C)c1ccc2c(c1)CCC1C(C)(CO)CCCC21C</chem>
Mol. weight [g/mol]:	286.45

Physical Properties

Property code	Value	Unit	Source
gf	150.02	kJ/mol	Joback Method
hf	-256.63	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	77.56	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.813		Crippen Method
mvol	253.050	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	803.21	K	Joback Method
tc	1023.32	K	Joback Method
tf	484.84	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.48	J/molxK	803.21	Joback Method
cpg	834.78	J/molxK	839.89	Joback Method
cpg	855.97	J/molxK	876.58	Joback Method
cpg	877.34	J/molxK	913.26	Joback Method
cpg	899.15	J/molxK	949.95	Joback Method
cpg	921.66	J/molxK	986.63	Joback Method
cpg	945.17	J/molxK	1023.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R291400&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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