Dehydroabienol

Inchi: InChI=1S/C20H32O/c1-7-15(2)9-10-17-19(5)13-8-12-18(3,4)16(19)11-14-20(17,6)21/h7,9
InchiKey: UUDIFKILZHQUQI-NAINOWQMSA-N
Formula: C20H32O
SMILES: C=CC(C)=CC=C1C(C)(O)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 288.47

Physical Properties

Property code	Value	Unit	Source
gf	226.88	kJ/mol	Joback Method
hf	-173.47	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.422		Crippen Method
mcvol	263.910	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	778.48	K	Joback Method
tc	995.75	K	Joback Method
tf	450.56	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.88	J/mol×K	778.48	Joback Method
cpg	851.63	J/mol×K	814.69	Joback Method
cpg	874.56	J/mol×K	850.90	Joback Method
cpg	898.02	J/mol×K	887.12	Joback Method
cpg	922.36	J/mol×K	923.33	Joback Method
cpg	947.93	J/mol×K	959.54	Joback Method
cpg	975.07	J/mol×K	995.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615366&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
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