Dehydroabietene

Inchi: InChI=1S/C20H30/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h8,13
InchiKey: CPKKFWRTJRSFHM-UHFFFAOYSA-N
Formula: C20H30
SMILES: C=C(C)C1=CC2=CCC3C(C)(C)CCCC3(C)C2CC1
Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	340.53	kJ/mol	Joback Method
hf	-50.13	kJ/mol	Joback Method
hfus	19.01	kJ/mol	Joback Method
hvap	59.42	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	6.062		Crippen Method
mcvol	247.180	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2029.00		NIST Webbook
tb	699.22	K	Joback Method
tc	936.76	K	Joback Method
tf	405.78	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.02	J/mol×K	699.22	Joback Method
cpg	766.27	J/mol×K	738.81	Joback Method
cpg	790.48	J/mol×K	778.40	Joback Method
cpg	814.02	J/mol×K	817.99	Joback Method
cpg	837.21	J/mol×K	857.58	Joback Method
cpg	860.40	J/mol×K	897.17	Joback Method
cpg	883.94	J/mol×K	936.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R266647&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

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