Abietal

Other names: Abietinal
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: HOFSYSONRIGEAC-TUNPWDSISA-N
Formula: C20H30O
SMILES: CC(C)C1=CC2=CCC3C(C)(C=O)CCCC3(C)C2CC1
Mol. weight [g/mol]: 286.45

Physical Properties

Property code	Value	Unit	Source
gf	159.28	kJ/mol	Joback Method
hf	-256.63	kJ/mol	Joback Method
hfus	20.37	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.321		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2267.00		NIST Webbook
ripol	2986.00		NIST Webbook
ripol	2959.00		NIST Webbook
ripol	2994.00		NIST Webbook
ripol	2959.00		NIST Webbook
ripol	2994.00		NIST Webbook
tb	750.88	K	Joback Method
tc	985.34	K	Joback Method
tf	448.50	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.64	J/mol×K	750.88	Joback Method
cpg	817.55	J/mol×K	789.96	Joback Method
cpg	840.83	J/mol×K	829.03	Joback Method
cpg	863.79	J/mol×K	868.11	Joback Method
cpg	886.76	J/mol×K	907.19	Joback Method
cpg	910.05	J/mol×K	946.26	Joback Method
cpg	933.99	J/mol×K	985.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R167169&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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