

Kaur-16-ene, (8«beta»,13«beta»)-

Other names:	8«beta»,13«beta»-Kaur-16-ene Phyllocladene, (-)- (-)-Phyllocladene
Inchi:	InChI=1S/C20H32/c1-14-12-20-11-8-16-18(2,3)9-5-10-19(16,4)17(20)7-6-15(14)13-20/h
InchiKey:	ONVABDHFQKWOSV-UHFFFAOYSA-N
Formula:	C20H32
SMILES:	C=C1CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]:	272.47
CAS:	20070-61-5

Physical Properties

Property code	Value	Unit	Source
gf	333.31	kJ/mol	Joback Method
hf	-100.29	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.975		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2012.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	2012.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	1971.00		NIST Webbook

ripol	1983.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2362.00		NIST Webbook
ripol	2319.00		NIST Webbook
tb	691.58	K	Joback Method
tc	933.36	K	Joback Method
tf	449.74	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.47	J/mol×K	691.58	Joback Method
cpg	795.89	J/mol×K	731.88	Joback Method
cpg	822.42	J/mol×K	772.17	Joback Method
cpg	848.59	J/mol×K	812.47	Joback Method
cpg	874.91	J/mol×K	852.76	Joback Method
cpg	901.90	J/mol×K	893.06	Joback Method
cpg	930.06	J/mol×K	933.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C20070615&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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