

Kaur-15-ene, (5«alpha»,9«alpha»,10«beta»)-

Other names:	Phylloclad-15-ene (+)-Isophyllocladene Isophyllocladen Isophyllocladene Isophyllocladene, (+)-
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:	DQUHDYWUEKWRLN-VYCOEXPQSA-N
Formula:	C20H32
SMILES:	CC1=CC2CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]:	272.47
CAS:	511-85-3

Physical Properties

Property code	Value	Unit	Source
gf	300.56	kJ/mol	Joback Method
hf	-138.22	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	57.34	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.975		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	2006.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1967.00		NIST Webbook
ripol	2238.00		NIST Webbook
ripol	2277.00		NIST Webbook
ripol	2238.00		NIST Webbook

tb	696.56	K	Joback Method
tc	939.38	K	Joback Method
tf	449.34	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.83	J/mol×K	696.56	Joback Method
cpg	797.09	J/mol×K	737.03	Joback Method
cpg	823.56	J/mol×K	777.50	Joback Method
cpg	849.75	J/mol×K	817.97	Joback Method
cpg	876.18	J/mol×K	858.44	Joback Method
cpg	903.39	J/mol×K	898.91	Joback Method
cpg	931.90	J/mol×K	939.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C511853&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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