Kaur-16-ene

Other names:	(-)-Kaur-16-ene
	(-)-Kaurene
	Ent-Kaur-16-ene
	Ent-Kaurene
	16-Kaurene
	Kauren-16-ene
	alpha-Kaurene
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/h1
InchiKey:	ONVABDHFQKWOSV-LAMXRXJRSA-N
Formula:	C20H32
SMILES:	C=C1CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]:	272.47
CAS:	562-28-7

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	2034.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2061.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2031.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2061.00		NIST Webbook
rinpol	2041.30		NIST Webbook

rinpol	2036.00		NIST Webbook
rinpol	2006.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2003.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2061.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2426.00		NIST Webbook
ripol	2426.00		NIST Webbook
tb	691.58	K	Joback Method
tc	933.36	K	Joback Method
tf	449.74	K	Joback Method
vc	0.927	m3/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/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=C562287&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