Kaur-15-ene

Other names:	(-)-Isokaurene
	Ent-15-Kaurene
	Isokauren
	Isokaurene
	Kryptomeren
	15-Kaurene
	Kauren-15-ene
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:	DQUHDYWUEKWRLN-UHFFFAOYSA-N
Formula:	C20H32
SMILES:	CC1=CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]:	272.47
CAS:	5947-50-2

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	1987.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1953.00		NIST Webbook

rinpol	1967.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2321.00		NIST Webbook
ripol	2346.00		NIST Webbook
tb	696.56	K	Joback Method
tc	939.38	K	Joback Method
tf	449.34	K	Joback Method
vc	0.929	m3/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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5947502&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