«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: DQUHDYWUEKWRLN-ZVWUZSKRSA-N
Formula: C20H32
SMILES: CC1=CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 272.47

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	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
ripol	2363.00		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=R518275&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