(4aS,5S,8aS)-5-Isopentyl-1,1,4a-trimethyl-6-methy

Inchi: InChI=1S/C19H34/c1-14(2)8-10-16-15(3)9-11-17-18(4,5)12-7-13-19(16,17)6/h14,16-17H
InchiKey: IGIFGCVMQOUKDF-LNLFQRSKSA-N
Formula: C19H34
SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)C
Mol. weight [g/mol]: 262.47
CAS: 220766-78-9

Physical Properties

Property code	Value	Unit	Source
gf	206.44	kJ/mol	Joback Method
hf	-245.77	kJ/mol	Joback Method
hfus	17.70	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	6.221		Crippen Method
mcvol	252.550	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	1803.60		NIST Webbook
tb	654.54	K	Joback Method
tc	867.39	K	Joback Method
tf	363.69	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.91	J/mol×K	654.54	Joback Method
cpg	766.39	J/mol×K	690.02	Joback Method
cpg	790.69	J/mol×K	725.49	Joback Method
cpg	814.04	J/mol×K	760.97	Joback Method
cpg	836.64	J/mol×K	796.44	Joback Method
cpg	858.72	J/mol×K	831.92	Joback Method
cpg	880.49	J/mol×K	867.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220766789&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume