(4aS,5S,8aS)-5-Isopentyl-1,1,4a,6-tetramethyl-1,2,3

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/h9,14,16-17
InchiKey: BMHNLNJEFVKDHC-LNLFQRSKSA-N
Formula: C19H34
SMILES: CC1=CCC2C(C)(C)CCCC2(C)C1CCC(C)C
Mol. weight [g/mol]: 262.47
CAS: 220766-81-4

Physical Properties

Property code	Value	Unit	Source
gf	173.69	kJ/mol	Joback Method
hf	-283.70	kJ/mol	Joback Method
hfus	19.69	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	6.221		Crippen Method
mcvol	252.550	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	1836.40		NIST Webbook
tb	659.52	K	Joback Method
tc	873.42	K	Joback Method
tf	363.29	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.60	J/mol×K	659.52	Joback Method
cpg	767.89	J/mol×K	695.17	Joback Method
cpg	792.05	J/mol×K	730.82	Joback Method
cpg	815.28	J/mol×K	766.47	Joback Method
cpg	837.82	J/mol×K	802.12	Joback Method
cpg	859.88	J/mol×K	837.77	Joback Method
cpg	881.68	J/mol×K	873.42	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=C220766814&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume