

(4aS,8aS)-8-Isopentyl-4,4,7,8a-tetramethyl-1,2,3,4,

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/h14,17H,7-
InchiKey:	XLWWCRFEOGZDEK-PKOBXYMFSA-N
Formula:	C19H34
SMILES:	CC1=C(CCC(C)C)C2(C)CCCC(C)(C)C2CC1
Mol. weight [g/mol]:	262.47
CAS:	220766-79-0

Physical Properties

Property code	Value	Unit	Source
gf	171.77	kJ/mol	Joback Method
hf	-274.83	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	57.02	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.366		Crippen Method
mcvol	252.550	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	1811.50		NIST Webbook
tb	669.17	K	Joback Method
tc	883.95	K	Joback Method
tf	380.05	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.05	J/molxK	669.17	Joback Method
cpg	766.67	J/molxK	704.97	Joback Method
cpg	790.25	J/molxK	740.76	Joback Method
cpg	813.02	J/molxK	776.56	Joback Method
cpg	835.19	J/molxK	812.35	Joback Method
cpg	857.00	J/molxK	848.15	Joback Method
cpg	878.66	J/molxK	883.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220766790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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