

CIS-1,2,2,3-TETRAMETHYLCYCLOPENTANE

Inchi:	InChI=1S/C9H18/c1-7-5-6-8(2)9(7,3)4/h7-8H,5-6H2,1-4H3
InchiKey:	DHLYDHNCPUAVHP-OCAPTIKFSA-N
Formula:	C9H18
SMILES:	CC1CCC(C)C1(C)C
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	40.54	kJ/mol	Joback Method
hf	-194.05	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	34.12	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mvol	126.810	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	411.50	K	Joback Method
tc	610.26	K	Joback Method
tf	217.51	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.44	J/mol×K	411.50	Joback Method
cpg	275.25	J/mol×K	444.63	Joback Method
cpg	292.94	J/mol×K	477.75	Joback Method
cpg	309.58	J/mol×K	510.88	Joback Method
cpg	325.27	J/mol×K	544.01	Joback Method
cpg	340.08	J/mol×K	577.14	Joback Method
cpg	354.09	J/mol×K	610.26	Joback Method

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=551
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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