

cis,cis,cis,trans-1,2,3,4-Tetramethylcyclopentane

Other names:	1-cis-2-cis-3-trans-4-tetramethylcyclopentane
Inchi:	InChI=1S/C9H18/c1-6-5-7(2)9(4)8(6)3/h6-9H,5H2,1-4H3/t6-,7-,8-,9+/m1/s1
InchiKey:	INYXDKODFMWKER-BGZDPUMWSA-N
Formula:	C9H18
SMILES:	CC1CC(C)C(C)C1C
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	38.32	kJ/mol	Joback Method
hf	-229.63	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	34.96	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.934		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	857.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	857.90		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	862.70		NIST Webbook
rinpol	862.00		NIST Webbook
tb	406.59	K	Joback Method
tc	596.26	K	Joback Method
tf	189.37	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.30	J/mol×K	406.59	Joback Method

cpg	273.56	J/mol×K	438.20	Joback Method
cpg	291.10	J/mol×K	469.81	Joback Method
cpg	307.92	J/mol×K	501.43	Joback Method
cpg	324.05	J/mol×K	533.04	Joback Method
cpg	339.49	J/mol×K	564.65	Joback Method
cpg	354.24	J/mol×K	596.26	Joback Method
dvisc	0.0006663	Pa×s	189.37	Joback Method
dvisc	0.0005055	Pa×s	225.57	Joback Method
dvisc	0.0004140	Pa×s	261.78	Joback Method
dvisc	0.0003559	Pa×s	297.98	Joback Method
dvisc	0.0003162	Pa×s	334.18	Joback Method
dvisc	0.0002875	Pa×s	370.39	Joback Method
dvisc	0.0002658	Pa×s	406.59	Joback Method

Sources

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=R92880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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