

1-cis-2-trans-3-cis-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-BZNPZCIMSА-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
mvol	126.810	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	871.10		NIST Webbook
rinpol	876.10		NIST Webbook
tb	406.59	K	Joback Method
tc	596.26	K	Joback Method
tf	189.37	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.30	J/molxK	406.59	Joback Method
cpg	339.49	J/molxK	564.65	Joback Method
cpg	324.05	J/molxK	533.04	Joback Method
cpg	307.92	J/molxK	501.43	Joback Method
cpg	291.10	J/molxK	469.81	Joback Method
cpg	273.56	J/molxK	438.20	Joback Method
cpg	354.24	J/molxK	596.26	Joback Method
dvisc	0.0002658	Paxs	406.59	Joback Method

dvisc	0.0002875	Paxs	370.39	Joback Method
dvisc	0.0003162	Paxs	334.18	Joback Method
dvisc	0.0003559	Paxs	297.98	Joback Method
dvisc	0.0004140	Paxs	261.78	Joback Method
dvisc	0.0005055	Paxs	225.57	Joback Method
dvisc	0.0006663	Paxs	189.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164482&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
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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