

1-trans-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-HXFLIBJXSA-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	829.40		NIST Webbook
rinpol	834.60		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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=R134733&Units=SI

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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