

1,2,3-Trimethylcyclohexane, cis, trans, cis

Inchi:

InChI=1S/C9H18/c1-7-5-4-6-8(2)9(7)3/h7-9H,4-6H2,1-3H3/t7-,8+,9+

InchiKey:

DQTVJLHNWPRPPH-BRPSZJMVSA-N

Formula:

C9H18

SMILES:

CC1CCCC(C)C1C

Mol. weight [g/mol]:

126.24

Physical Properties

Property code	Value	Unit	Source
gf	33.93	kJ/mol	Joback Method
hf	-215.45	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	35.44	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	867.00		NIST Webbook
tb	415.53	K	Joback Method
tc	613.57	K	Joback Method
tf	190.09	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.82	J/mol×K	415.53	Joback Method
cpg	273.92	J/mol×K	448.54	Joback Method
cpg	292.21	J/mol×K	481.54	Joback Method
cpg	309.72	J/mol×K	514.55	Joback Method
cpg	326.43	J/mol×K	547.56	Joback Method
cpg	342.37	J/mol×K	580.57	Joback Method
cpg	357.55	J/mol×K	613.57	Joback Method
dvisc	0.0024227	Pa×s	190.09	Joback Method
dvisc	0.0012236	Pa×s	227.66	Joback Method

dvisc	0.0007500	Pa×s	265.24	Joback Method
dvisc	0.0005190	Pa×s	302.81	Joback Method
dvisc	0.0003896	Pa×s	340.38	Joback Method
dvisc	0.0003096	Pa×s	377.96	Joback Method
dvisc	0.0002565	Pa×s	415.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R595232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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