

1,2,4-Trimethylcyclohexane, cis,trans,trans

Inchi:	InChI=1S/C9H18/c1-7-4-5-8(2)9(3)6-7/h7-9H,4-6H2,1-3H3/t7-,8-,9-/m1/s1
InchiKey:	VCJPCEVERINRSG-IWSPIIDZSA-N
Formula:	C9H18
SMILES:	CC1CCC(C)C(C)C1
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	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
tb	415.53	K	Joback Method
tc	613.57	K	Joback Method
tf	190.09	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.82	J/molxK	415.53	Joback Method
cpg	273.92	J/molxK	448.54	Joback Method
cpg	292.21	J/molxK	481.54	Joback Method
cpg	309.72	J/molxK	514.55	Joback Method
cpg	326.43	J/molxK	547.56	Joback Method
cpg	342.37	J/molxK	580.57	Joback Method
cpg	357.55	J/molxK	613.57	Joback Method
dvisc	0.0024227	Paxs	190.09	Joback Method

dvisc	0.0012236	Paxs	227.66	Joback Method
dvisc	0.0007500	Paxs	265.24	Joback Method
dvisc	0.0005190	Paxs	302.81	Joback Method
dvisc	0.0003896	Paxs	340.38	Joback Method
dvisc	0.0003096	Paxs	377.96	Joback Method
dvisc	0.0002565	Paxs	415.53	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=R595247&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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