

Cyclohexane, 1,2,4-trimethyl-

Other names:	1,2,4-trimethylcyclohexane 1,3,4-trimethylcyclohexane
Inchi:	InChI=1S/C9H18/c1-7-4-5-8(2)9(3)6-7/h7-9H,4-6H2,1-3H3
InchiKey:	VCJPCEVERINRSG-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC1CCC(C)C(C)C1
Mol. weight [g/mol]:	126.24
CAS:	2234-75-5

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
ie	9.38	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	847.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	844.40		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	881.00		NIST Webbook
tb	415.53	K	Joback Method
tc	613.57	K	Joback Method
tf	186.75 ± 0.50	K	NIST Webbook
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	0.0002565	Paxs	415.53	Joback Method
dvisc	0.0012236	Paxs	227.66	Joback Method
dvisc	0.0007500	Paxs	265.24	Joback Method
dvisc	0.0024227	Paxs	190.09	Joback Method
dvisc	0.0003896	Paxs	340.38	Joback Method
dvisc	0.0003096	Paxs	377.96	Joback Method
dvisc	0.0005190	Paxs	302.81	Joback Method
rhol	790.80	kg/m3	293.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rhol	786.92	kg/m3	298.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rhol	783.03	kg/m3	303.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rhol	779.13	kg/m3	308.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes

rho_l	775.23	kg/m ³	313.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rho_l	771.32	kg/m ³	318.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes

Sources

Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes.
McGowan Method:

<https://www.doi.org/10.1021/je400529k>

NIST Webbook:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2234755&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rho_l:	Liquid Density
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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