

1,3-Dimethylcyclohexane

Other names:	1,3-Dimethylcyclohexane cis-trans 1,3-Dimethylcyclohexane,c&t UN 2263 cis,trans-1,3-Dimethylcyclohexane cyclohexane, 1,3-dimethyl- hexahydro-m-xylene m-dimethylcyclohexane
Inchi:	InChI=1S/C8H16/c1-7-4-3-5-8(2)6-7/h7-8H,3-6H2,1-2H3
InchiKey:	SGVUHPSBDNVHKL-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC1CCCC(C)C1
Mol. weight [g/mol]:	112.22
CAS:	591-21-9

Physical Properties

Property code	Value	Unit	Source
af	0.2555		Cheméo Relay (1.0)
chl	-5221.60	kJ/mol	NIST Webbook
gf	33.22	kJ/mol	Joback Method
hf	-164.18	kJ/mol	Cheméo Relay (1.0)
hfus	9.38	kJ/mol	Joback Method
hvap	35.98	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-4.58		Cheméo Relay (1.0)
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	775.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	806.00		NIST Webbook

rinpol	787.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	785.00		NIST Webbook
ripol	814.00		NIST Webbook
ripol	860.00		NIST Webbook
ripol	860.00		NIST Webbook
tb	392.00 ± 3.00	K	NIST Webbook
tb	392.70 ± 2.00	K	NIST Webbook
tb	394.00 ± 2.00	K	NIST Webbook
tb	395.00 ± 3.00	K	NIST Webbook
tb	393.00 ± 3.00	K	NIST Webbook
tb	393.00 ± 5.00	K	NIST Webbook
tb	383.00 ± 15.00	K	NIST Webbook
tb	443.00 ± 5.00	K	NIST Webbook
tb	390.00 ± 6.00	K	NIST Webbook
tb	391.00 ± 5.00	K	NIST Webbook
tb	391.20 ± 4.00	K	NIST Webbook
tb	395.00 ± 6.00	K	NIST Webbook
tb	392.00 ± 6.00	K	NIST Webbook
tb	391.00 ± 6.00	K	NIST Webbook
tb	390.00 ± 6.00	K	NIST Webbook
tb	391.00 ± 2.00	K	NIST Webbook
tb	395.70	K	NIST Webbook
tb	393.00 ± 5.00	K	NIST Webbook
tb	392.00 ± 4.00	K	NIST Webbook
tb	389.65 ± 2.00	K	NIST Webbook
tb	394.70 ± 1.50	K	NIST Webbook
tb	394.70 ± 1.00	K	NIST Webbook
tb	394.85 ± 3.00	K	NIST Webbook
tb	394.90 ± 2.00	K	NIST Webbook
tb	395.00 ± 1.50	K	NIST Webbook
tb	394.65 ± 0.60	K	NIST Webbook
tb	393.90 ± 0.50	K	NIST Webbook
tc	584.50	K	Cheméo Relay (1.0)
tf	168.94	K	Cheméo Relay (1.0)
vc	0.404	m ³ /kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.54	J/mol×K	397.32	Joback Method

cpg	307.47	J/mol×K	597.67	Joback Method
cpg	293.52	J/mol×K	564.28	Joback Method
cpg	278.84	J/mol×K	530.89	Joback Method
cpg	263.41	J/mol×K	497.49	Joback Method
cpg	247.23	J/mol×K	464.10	Joback Method
cpg	230.28	J/mol×K	430.71	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0002631	Pa×s	397.32	Joback Method
dvisc	0.0003324	Pa×s	361.61	Joback Method
dvisc	0.0004419	Pa×s	325.90	Joback Method
dvisc	0.0041986	Pa×s	183.06	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
dvisc	0.0018154	Pa×s	218.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42809e+01
Coeff. B	-3.31009e+03
Coeff. C	-5.04320e+01
Temperature range (K), min.	286.98
Temperature range (K), max.	419.47

Sources

The Yaws Handbook of Vapor

Pressure:

NIST Webbook:

McGowan Method:

Miscibility behavior of

triethyl(tetradecyl)phosphonium

iodide with cyclic

hydrocarbons:

Cheméo Relay (1.0):

Crippen Method:

Crippen Method:

Cheméo Relay (1.0, beta):

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C591219&Units=SI>

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

<https://www.doi.org/10.1016/j.fluid.2014.03.020>

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

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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