

Cyclohexene, 1,4-dimethyl-

Other names:	1,4-Dimethyl-1-cyclohexene 1,4-Dimethylcyclohexene
Inchi:	InChI=1S/C8H14/c1-7-3-5-8(2)6-4-7/h3,8H,4-6H2,1-2H3
InchiKey:	KMGDYKOGDOVDCW-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC1=CCC(C)CC1
Mol. weight [g/mol]:	110.20
CAS:	2808-79-9

Physical Properties

Property code	Value	Unit	Source
gf	61.26	kJ/mol	Joback Method
hf	-107.82	kJ/mol	Joback Method
hfus	9.14	kJ/mol	Joback Method
hvap	34.79	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.753		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	825.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	826.70		NIST Webbook
rinpol	825.00		NIST Webbook
ripol	946.00		NIST Webbook
ripol	946.00		NIST Webbook
tb	398.00 ± 3.00	K	NIST Webbook
tb	398.00 ± 3.00	K	NIST Webbook
tc	610.71	K	Joback Method
tf	213.75 ± 0.50	K	NIST Webbook
vc	0.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.81	J/molxK	406.13	Joback Method
cpg	273.11	J/molxK	576.61	Joback Method
cpg	260.26	J/molxK	542.51	Joback Method
cpg	246.71	J/molxK	508.42	Joback Method
cpg	232.47	J/molxK	474.32	Joback Method
cpg	217.51	J/molxK	440.23	Joback Method
cpg	285.31	J/molxK	610.71	Joback Method
dvisc	0.0002466	Paxs	406.13	Joback Method
dvisc	0.0003123	Paxs	371.87	Joback Method
dvisc	0.0004149	Paxs	337.61	Joback Method
dvisc	0.0005878	Paxs	303.36	Joback Method
dvisc	0.0009098	Paxs	269.10	Joback Method
dvisc	0.0015996	Paxs	234.84	Joback Method
dvisc	0.0034105	Paxs	200.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41175e+01
Coeff. B	-3.22526e+03
Coeff. C	-5.84700e+01
Temperature range (K), min.	291.68
Temperature range (K), max.	424.73

Sources

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=C2808799&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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