

Cyclohexene, 1,5-dimethyl-

Other names:	1,5-dimethylcyclohexene
Inchi:	InChI=1S/C8H14/c1-7-4-3-5-8(2)6-7/h4,8H,3,5-6H2,1-2H3
InchiKey:	QOSLKKIVSIPIFE-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC1=CCCC(C)C1
Mol. weight [g/mol]:	110.20
CAS:	2808-77-7

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	829.00		NIST Webbook
rinpol	825.00		NIST Webbook
tb	402.00 ± 4.00	K	NIST Webbook
tb	398.00 ± 4.00	K	NIST Webbook
tb	400.80 ± 2.00	K	NIST Webbook
tc	610.71	K	Joback Method
tf	200.58	K	Joback Method
vc	0.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.81	J/mol×K	406.13	Joback Method
cpg	217.51	J/mol×K	440.23	Joback Method
cpg	232.47	J/mol×K	474.32	Joback Method

cpg	246.71	J/mol×K	508.42	Joback Method
cpg	260.26	J/mol×K	542.51	Joback Method
cpg	273.11	J/mol×K	576.61	Joback Method
cpg	285.31	J/mol×K	610.71	Joback Method
dvisc	0.0034105	Paxs	200.58	Joback Method
dvisc	0.0015996	Paxs	234.84	Joback Method
dvisc	0.0009098	Paxs	269.10	Joback Method
dvisc	0.0005878	Paxs	303.36	Joback Method
dvisc	0.0004149	Paxs	337.61	Joback Method
dvisc	0.0003123	Paxs	371.87	Joback Method
dvisc	0.0002466	Paxs	406.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37449e+01
Coeff. B	-3.13526e+03
Coeff. C	-5.84700e+01
Temperature range (K), min.	291.45
Temperature range (K), max.	430.23

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2808777&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/19-592-4/Cyclohexene-1-5-dimethyl.pdf>

Generated by Cheméo on 2024-04-26 10:45:48.198933443 +0000 UTC m=+16417597.119510756.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.