

1,4-Dimethyl cyclohexene

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:	70688-47-0

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
tb	406.13	K	Joback Method
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/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

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=C70688470&Units=SI
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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