1,3-Dimethyl-1-cyclohexene

Other names: 1,3-Dimethyl cyclohexene
Cyclohexene, 1,3-dimethyl-
1,3-Dimethyl-3-cyclohexene
Inchi: InChI=1S/C8H14/c1-7-4-3-5-8(2)6-7/h6-7H,3-5H2,1-2H3
InchiKey: XTCMQAVNRXZBRH-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC1=CC(C)CCC1
Mol. weight [g/mol]: 110.20
CAS: 2808-76-6

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	836.00		NIST Webbook
rinpol	825.00		NIST Webbook
tb	397.00 ± 3.00	K	NIST Webbook
tb	398.00 ± 3.00	K	NIST Webbook
tb	400.20	K	NIST Webbook
tb	398.00 ± 4.00	K	NIST Webbook
tc	610.71	K	Joback Method
tf	200.58	K	Joback Method
vc	0.403	m3/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	Pa×s	200.58	Joback Method
dvisc	0.0015996	Pa×s	234.84	Joback Method
dvisc	0.0009098	Pa×s	269.10	Joback Method
dvisc	0.0005878	Pa×s	303.36	Joback Method
dvisc	0.0004149	Pa×s	337.61	Joback Method
dvisc	0.0003123	Pa×s	371.87	Joback Method
dvisc	0.0002466	Pa×s	406.13	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2808766&Units=SI

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

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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