

Cyclohexane, 1-(1,1-dimethylethyl)-4-methyl-

Inchi:	InChI=1S/C11H22/c1-9-5-7-10(8-6-9)11(2,3)4/h9-10H,5-8H2,1-4H3
InchiKey:	YCLKWKCHQLIGTA-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CC1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]:	154.29
CAS:	75736-66-2

Physical Properties

Property code	Value	Unit	Source
gf	61.32	kJ/mol	Joback Method
hf	-245.14	kJ/mol	Joback Method
hfus	9.74	kJ/mol	Joback Method
hvap	38.90	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.859		Crippen Method
mvol	154.990	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
tb	459.87 ± 1.00	K	NIST Webbook
tb	461.89 ± 1.00	K	NIST Webbook
tc	669.86	K	Joback Method
tf	219.29	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.39	J/mol×K	462.73	Joback Method
cpg	370.79	J/mol×K	497.25	Joback Method
cpg	391.96	J/mol×K	531.77	Joback Method
cpg	411.95	J/mol×K	566.30	Joback Method
cpg	430.80	J/mol×K	600.82	Joback Method
cpg	448.56	J/mol×K	635.34	Joback Method
cpg	465.26	J/mol×K	669.86	Joback Method
dvisc	0.0086592	Paxs	219.29	Joback Method

dvisc	0.0030549	Paxs	259.86	Joback Method
dvisc	0.0014280	Paxs	300.44	Joback Method
dvisc	0.0007999	Paxs	341.01	Joback Method
dvisc	0.0005069	Paxs	381.58	Joback Method
dvisc	0.0003506	Paxs	422.16	Joback Method
dvisc	0.0002587	Paxs	462.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C75736662&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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