Cyclohexane, (1,1-dimethylpropyl)-

Other names:	Cyclohexane, tert-pentyl-
	tert-Pentylcyclohexane
	2-Cyclohexyl-2-methylbutane
	2-Methyl-2-cyclohexylbutane
	t-Pentylcyclohexane
Inchi:	InChI=1S/C11H22/c1-4-11(2,3)10-8-6-5-7-9-10/h10H,4-9H2,1-3H3
InchiKey:	HEOYZKPYPRYIAR-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CCC(C)(C)C1CCCCC1
Mol. weight [g/mol]:	154.29
CAS:	31797-64-5

Physical Properties

Property code	Value	Unit	Source
gf	69.03	kJ/mol	Joback Method
hf	-224.80	kJ/mol	Joback Method
hfus	8.67	kJ/mol	Joback Method
hvap	39.21	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	4.003		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	471.55 ± 0.40	K	NIST Webbook
tb	471.23 ± 0.50	K	NIST Webbook
tb	471.23 ± 0.50	K	NIST Webbook
tb	465.00 ± 5.00	K	NIST Webbook
tc	674.83	K	Joback Method
tf	223.53	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.70	J/mol×K	467.40	Joback Method
cpg	446.70	J/mol×K	640.26	Joback Method
cpg	429.41	J/mol×K	605.69	Joback Method
cpg	411.01	J/mol×K	571.11	Joback Method
cpg	391.46	J/mol×K	536.54	Joback Method
cpg	370.71	J/mol×K	501.97	Joback Method
cpg	462.94	J/mol×K	674.83	Joback Method
dvisc	0.0002509	Pa×s	467.40	Joback Method
dvisc	0.0003556	Pa×s	426.75	Joback Method
dvisc	0.0005423	Pa×s	386.11	Joback Method
dvisc	0.0009134	Pa×s	345.46	Joback Method
dvisc	0.0017679	Pa×s	304.82	Joback Method
dvisc	0.0041931	Pa×s	264.18	Joback Method
dvisc	0.0136145	Pa×s	223.53	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=C31797645&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