Cyclohexane, (1-methylpropyl)-

Other names:	(1-METHYLPROPYL)CYCLOHEXANE
	2-CYCLOHEXYLBUTANE
	Cyclohexane, sec-butyl-
	SEC-BUTYLCYCLOHEXANE
	s-Butylcyclohexane
Inchi:	InChI=1S/C10H20/c1-3-9(2)10-7-5-4-6-8-10/h9-10H,3-8H2,1-2H3
InchiKey:	QTYARKOMFKRPSY-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CCC(C)C1CCCCC1
Mol. weight [g/mol]:	140.27
CAS:	7058-01-7

Physical Properties

Property code	Value	Unit	Source
af	0.2640		KDB
gf	55.33	kJ/mol	Joback Method
hf	-200.69	kJ/mol	Joback Method
hfus	9.97	kJ/mol	Joback Method
hvap	37.90	kJ/mol	Joback Method
ie	9.51 ± 0.03	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
log10ws	-3.42		Crippen Method
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2670.00	kPa	KDB
rinpol	1022.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1023.35		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1023.35		NIST Webbook
rinpol	1032.00		NIST Webbook

rinpol	1014.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1120.00		NIST Webbook
tb	450.30 ± 0.50	K	NIST Webbook
tb	452.50	K	KDB
tb	452.48 ± 0.03	K	NIST Webbook
tb	452.90 ± 0.50	K	NIST Webbook
tb	452.20 ± 2.00	K	NIST Webbook
tb	452.50	K	NIST Webbook
tc	669.00	K	KDB
tf	194.84	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.89	J/mol×K	648.75	Joback Method
cpg	299.96	J/mol×K	447.31	Joback Method
cpg	319.98	J/mol×K	480.88	Joback Method
cpg	339.02	J/mol×K	514.46	Joback Method
cpg	357.11	J/mol×K	548.03	Joback Method
cpg	374.26	J/mol×K	581.60	Joback Method
cpg	390.52	J/mol×K	615.17	Joback Method
dvisc	0.0002520	Pa×s	447.31	Joback Method
dvisc	0.0151535	Pa×s	194.84	Joback Method
dvisc	0.0041753	Pa×s	236.92	Joback Method
dvisc	0.0016972	Pa×s	279.00	Joback Method
dvisc	0.0008734	Pa×s	321.07	Joback Method
dvisc	0.0005243	Pa×s	363.15	Joback Method
dvisc	0.0003499	Pa×s	405.23	Joback Method
hvapt	44.10	kJ/mol	412.00	NIST Webbook
rhol	813.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44336e+01
Coeff. B	-3.78447e+03
Coeff. C	-6.69310e+01
Temperature range (K), min.	334.46
Temperature range (K), max.	481.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.95636e+01
Coeff. B	-9.44578e+03
Coeff. C	-1.22948e+01
Coeff. D	5.39976e-06
Temperature range (K), min.	364.15
Temperature range (K), max.	663.00

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7058017&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=586

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=586

Legend

af: Acentric Factor

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume