Cyclohexane, (2-methylpropyl)-

Other names:	(2-METHYLPROPYL)CYCLOHEXANE
	(2-Methyl-propyl)-cyclohexane
	2-methylpropylcyclohexane
	Cyclohexane, isobutyl-
	I-BUTYLCYCLOHEXANE
	Isobutylcyclohexane
	cyclohexane, 2-methylpropyl-
Inchi:	InChI=1S/C10H20/c1-9(2)8-10-6-4-3-5-7-10/h9-10H,3-8H2,1-2H3
InchiKey:	FFROMNOQCNVNIH-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CC(C)CC1CCCCC1
Mol. weight [g/mol]:	140.27
CAS:	1678-98-4

Physical Properties

Property code	Value	Unit	Source
af	0.3190		KDB
gf	55.33	kJ/mol	Joback Method
hf	-200.69	kJ/mol	Joback Method
hfus	9.97	kJ/mol	Joback Method
hvap	47.50	kJ/mol	NIST Webbook
hvap	47.55	kJ/mol	NIST Webbook
ie	9.54 ± 0.03	eV	NIST Webbook
log10ws	-3.42		Crippen Method
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	3120.00	kPa	KDB
rinpol	1005.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	986.45		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	986.45		NIST Webbook
rinpol	1019.10		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1008.90		NIST Webbook

ripol	1058.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1058.00		NIST Webbook
tb	444.50	K	KDB
tc	659.00	K	KDB
tc	642.10	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
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	43.50	kJ/mol	400.50	NIST Webbook
rhol	795.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31070e+01
Coeff. B	-3.07023e+03
Coeff. C	-8.27550e+01
Temperature range (K), min.	322.25
Temperature range (K), max.	476.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.00618e+02
Coeff. B	-9.20294e+03
Coeff. C	-1.25726e+01
Coeff. D	6.88404e-06
Temperature range (K), min.	358.00
Temperature range (K), max.	659.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=585
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1678984&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
KDB:	https://www.cheric.org/files/research/kdb/mol/mol585.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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