Cyclohexane, bromo-

Other names:	1-Bromocyclohexane
	Bromocyclohexane
	Cyclohexyl bromide
Inchi:	InChI=1S/C6H11Br/c7-6-4-2-1-3-5-6/h6H,1-5H2
InchiKey:	AQNQQHJNRPDOQV-UHFFFAOYSA-N
Formula:	C6H11Br
SMILES:	BrC1CCCCC1
Mol. weight [g/mol]:	163.06
CAS:	108-85-0

Physical Properties

Property code	Value	Unit	Source
gf	38.41	kJ/mol	Joback Method
hf	-86.52	kJ/mol	Joback Method
hfus	8.42	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
ie	9.90 ± 0.02	eV	NIST Webbook
ie	9.87 ± 0.02	eV	NIST Webbook
ie	9.85 ± 0.01	eV	NIST Webbook
log10ws	-2.30		Aqueous Solubility Prediction Method
logp	2.714		Crippen Method
mcvol	102.040	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
rinpol	1009.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	975.00		NIST Webbook

rinpol	1023.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1288.00		NIST Webbook
tb	437.00 ± 1.00	K	NIST Webbook
tb	436.00 ± 4.00	K	NIST Webbook
tb	439.50 ± 0.50	K	NIST Webbook
tb	439.40	K	NIST Webbook
tb	438.00	K	NIST Webbook
tc	648.68	K	Joback Method
tf	206.00 ± 6.00	K	NIST Webbook
tf	216.40	K	Aqueous Solubility Prediction Method
tt	216.87 ± 0.05	K	NIST Webbook
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.89	J/mol×K	573.25	Joback Method
cpg	218.62	J/mol×K	535.53	Joback Method
cpg	253.12	J/mol×K	648.68	Joback Method
cpg	242.38	J/mol×K	610.96	Joback Method
cpg	176.75	J/mol×K	422.39	Joback Method
cpg	191.58	J/mol×K	460.10	Joback Method
cpg	205.53	J/mol×K	497.82	Joback Method
cpl	182.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0003921	Pa×s	422.39	Joback Method
dvisc	0.0009937	Pa×s	323.48	Joback Method
dvisc	0.0006882	Pa×s	356.45	Joback Method
dvisc	0.0005072	Pa×s	389.42	Joback Method
dvisc	0.0057128	Pa×s	224.56	Joback Method
dvisc	0.0027467	Pa×s	257.53	Joback Method
dvisc	0.0015594	Pa×s	290.50	Joback Method
hfust	10.79	kJ/mol	216.90	NIST Webbook
hfust	10.79	kJ/mol	216.90	NIST Webbook
hvapt	42.80	kJ/mol	393.00	NIST Webbook

rhol	1328.41	kg/m3	298.15	Study of the Surface Tension of Chlorocyclohexane or Bromocyclohexane with Some Cyclic Ethers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.00	K	4.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Study of the Surface Tension of Chlorocyclohexane or Bromocyclohexane with Some Cyclic Ethers:	https://www.doi.org/10.1021/je0500577
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume