Cyclohexene, 3-bromo-

Other names:	1-Bromo-2-cyclohexene
	2-Cyclohexen-1-yl bromide
	3-Bromo-1-cyclohexene
	3-Bromocyclohexene
	2-Cyclohexenyl bromide
Inchi:	InChI=1S/C6H9Br/c7-6-4-2-1-3-5-6/h2,4,6H,1,3,5H2
InchiKey:	AJKDUJRRWLQXHM-UHFFFAOYSA-N
Formula:	C6H9Br
SMILES:	BrC1C=CCCC1
Mol. weight [g/mol]:	161.04
CAS:	1521-51-3

Physical Properties

Property code	Value	Unit	Source
gf	68.37	kJ/mol	Joback Method
hf	-28.74	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	36.11	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.490		Crippen Method
mcvol	97.740	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	974.00		NIST Webbook
tb	421.55	K	Joback Method
tc	650.33	K	Joback Method
tf	225.32	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.16	J/mol×K	421.55	Joback Method
cpg	176.55	J/mol×K	459.68	Joback Method
cpg	189.10	J/mol×K	497.81	Joback Method

cpg	200.82	J/mol×K	535.94	Joback Method
cpg	211.77	J/mol×K	574.07	Joback Method
cpg	221.97	J/mol×K	612.20	Joback Method
cpg	231.47	J/mol×K	650.33	Joback Method
dvisc	0.0043841	Pa×s	225.32	Joback Method
dvisc	0.0022463	Pa×s	258.02	Joback Method
dvisc	0.0013378	Pa×s	290.73	Joback Method
dvisc	0.0008848	Pa×s	323.43	Joback Method
dvisc	0.0006314	Pa×s	356.14	Joback Method
dvisc	0.0004768	Pa×s	388.84	Joback Method
dvisc	0.0003761	Pa×s	421.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.50 ± 0.50	K	2.00	NIST Webbook
tbrp	329.50 ± 0.50	K	1.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1521513&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume