Cyclohexene, 1-bromo-

Other names: 1-bromocyclohex-1-ene
Inchi: InChI=1S/C6H9Br/c7-6-4-2-1-3-5-6/h4H,1-3,5H2
InchiKey: QBUMXSSCYUMVAW-UHFFFAOYSA-N
Formula: C6H9Br
SMILES: BrC1=CCCCC1
Mol. weight [g/mol]: 161.04
CAS: 2044-08-8

Physical Properties

Property code	Value	Unit	Source
gf	66.45	kJ/mol	Joback Method
hf	-19.87	kJ/mol	Joback Method
hfus	8.18	kJ/mol	Joback Method
hvap	37.08	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.839		Crippen Method
mcvol	97.740	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1324.00		NIST Webbook
tb	431.20	K	Joback Method
tc	661.96	K	Joback Method
tf	242.08	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.19	J/mol×K	431.20	Joback Method
cpg	217.97	J/mol×K	623.50	Joback Method
cpg	208.48	J/mol×K	585.04	Joback Method

cpg	198.30	J/mol×K	546.58	Joback Method
cpg	187.38	J/mol×K	508.12	Joback Method
cpg	175.69	J/mol×K	469.66	Joback Method
cpg	226.80	J/mol×K	661.96	Joback Method
dvisc	0.0003605	Pa×s	431.20	Joback Method
dvisc	0.0004644	Pa×s	399.68	Joback Method
dvisc	0.0006248	Pa×s	368.16	Joback Method
dvisc	0.0008887	Pa×s	336.64	Joback Method
dvisc	0.0013594	Pa×s	305.12	Joback Method
dvisc	0.0022933	Pa×s	273.60	Joback Method
dvisc	0.0044334	Pa×s	242.08	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2044088&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume