Benzene, 1-bromo-4-chloro-

Other names:	1-Bromo-4-chlorobenzene
	1-Chloro-4-bromobenzene
	4-Bromochlorobenzene
	4-Chloro-1-bromobenzene
	4-Chlorobromobenzene
	4-Chlorophenyl bromide
	NSC 17587
	benzene, 4-chlorobromo-
	p-Bromochlorobenzene
	p-Bromophenyl chloride
	p-Chlorobromobenzene
	p-Chlorophenyl bromide
Inchi:	InChI=1S/C6H4BrCl/c7-5-1-3-6(8)4-2-5/h1-4H
InchiKey:	NHDODQWIKUYWMW-UHFFFAOYSA-N
Formula:	C6H4BrCl
SMILES:	Clc1ccc(Br)cc1
Mol. weight [g/mol]:	191.45
CAS:	106-39-8

Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	68.48	kJ/mol	Joback Method
hfl	28.00	kJ/mol	NIST Webbook
hfus	19.90	kJ/mol	Synthesis and characterization of novel binary organic monotectic and eutectic alloys
hsub	69.10 ± 0.20	kJ/mol	NIST Webbook
hsub	69.30 ± 0.40	kJ/mol	NIST Webbook
hsub	69.34 ± 0.11	kJ/mol	NIST Webbook
hvap	42.71	kJ/mol	Joback Method
ie	9.04	eV	NIST Webbook
log10ws	-3.63		Aqueous Solubility Prediction Method
log10ws	-3.63		Estimated Solubility Method
logp	3.103		Crippen Method

mcvol	101.380	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
rinpol	1086.90		NIST Webbook
rinpol	188.00		NIST Webbook
tb	469.00	K	NIST Webbook
tb	469.20	K	NIST Webbook
tc	716.18	K	Joback Method
tf	339.82	K	Aqueous Solubility Prediction Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.69	J/mol×K	471.93	Joback Method
cpg	197.22	J/mol×K	716.18	Joback Method
cpg	172.55	J/mol×K	553.35	Joback Method
cpg	179.54	J/mol×K	594.05	Joback Method
cpg	185.95	J/mol×K	634.76	Joback Method
cpg	191.83	J/mol×K	675.47	Joback Method
cpg	164.95	J/mol×K	512.64	Joback Method
dvisc	0.0004080	Pa×s	440.95	Joback Method
dvisc	0.0005111	Pa×s	409.97	Joback Method
dvisc	0.0006641	Pa×s	378.99	Joback Method
dvisc	0.0009042	Pa×s	348.00	Joback Method
dvisc	0.0013076	Pa×s	317.02	Joback Method
dvisc	0.0003355	Pa×s	471.93	Joback Method
dvisc	0.0020482	Pa×s	286.04	Joback Method
hfust	18.40	kJ/mol	178.00	NIST Webbook
hfust	18.76	kJ/mol	337.75	NIST Webbook
hfust	18.76	kJ/mol	337.80	NIST Webbook
hsubt	67.90 ± 0.80	kJ/mol	315.50	NIST Webbook
hsubt	67.90 ± 0.40	kJ/mol	316.00	NIST Webbook
hvapt	49.10	kJ/mol	401.50	NIST Webbook
hvapt	49.70	kJ/mol	387.50	NIST Webbook
sfust	55.50	J/mol×K	337.75	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Synthesis and characterization of novel binary organic monotectic and eutectic alloys:	https://www.doi.org/10.1016/j.tca.2012.02.020
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume