Phenol, 4-bromo-

Other names:	4-Bromophenol
	Phenol, p-bromo-
	p-Bromophenol
	p-bromohydroxybenzene
	p-bromophenic acid
Inchi:	InChI=1S/C6H5BrO/c7-5-1-3-6(8)4-2-5/h1-4,8H
InchiKey:	GZFGOTFRPZRKDS-UHFFFAOYSA-N
Formula:	C6H5BrO
SMILES:	Oc1ccc(Br)cc1
Mol. weight [g/mol]:	173.01
CAS:	106-41-2

Physical Properties

Property code	Value	Unit	Source
gf	-28.25	kJ/mol	Joback Method
hf	-81.62	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hsub	83.10 ± 1.60	kJ/mol	NIST Webbook
hsub	87.30 ± 0.40	kJ/mol	NIST Webbook
hvap	50.67	kJ/mol	Joback Method
ie	8.52	eV	NIST Webbook
log10ws	-1.09		Aqueous Solubility Prediction Method
log10ws	-1.09		Estimated Solubility Method
logp	2.155		Crippen Method
mcvol	95.010	ml/mol	McGowan Method
pc	6451.51	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook

rinpol	1297.20		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	508.70	K	NIST Webbook
tb	511.20	K	NIST Webbook
tc	761.97	K	Joback Method
tf	337.80	K	Crystalline and liquid vapour pressures of the four p-monohalophenols: A thermodynamic study of their phase transitions
tf	336.00 ± 1.00	K	NIST Webbook
tf	337.87	K	Aqueous Solubility Prediction Method
tf	337.00 ± 2.00	K	NIST Webbook
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.59	J/mol×K	761.97	Joback Method
cpg	209.39	J/mol×K	720.00	Joback Method
cpg	203.78	J/mol×K	678.02	Joback Method
cpg	197.65	J/mol×K	636.05	Joback Method
cpg	190.89	J/mol×K	594.08	Joback Method
cpg	183.39	J/mol×K	552.11	Joback Method
cpg	175.03	J/mol×K	510.14	Joback Method
cpl	230.00	J/mol×K	337.00	NIST Webbook
cps	192.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0012814	Pa×s	381.12	Joback Method
dvisc	0.0006917	Pa×s	406.93	Joback Method
dvisc	0.0004018	Pa×s	432.73	Joback Method
dvisc	0.0001613	Pa×s	484.34	Joback Method
dvisc	0.0002481	Pa×s	458.53	Joback Method
dvisc	0.0001095	Pa×s	510.14	Joback Method
dvisc	0.0025966	Pa×s	355.32	Joback Method
hfust	16.57	kJ/mol	336.00	NIST Webbook
hfust	13.00	kJ/mol	3367.00	NIST Webbook
hfust	16.57	kJ/mol	336.00	NIST Webbook
hfust	16.57	kJ/mol	336.00	NIST Webbook
hfust	17.60	kJ/mol	338.20	NIST Webbook
hvapt	58.80	kJ/mol	450.50	NIST Webbook
sfust	49.30	J/mol×K	336.00	NIST Webbook

sfust	39.00	J/mol×K	3367.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crystalline and liquid vapour pressures of the four p-monohalophenols: A thermodynamic study of their phase transitions:	https://www.doi.org/10.1016/j.jct.2013.05.047
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106412&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid 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
hsub:	Enthalpy of sublimation 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
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

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