Phenol, 2-bromo-

Other names: Phenol, o-bromo-
o-Bromophenol
2-Bromophenol
2-Bromfenol
Inchi: InChI=1S/C6H5BrO/c7-5-3-1-2-4-6(5)8/h1-4,8H
InchiKey: VADKRMSMGWJZCF-UHFFFAOYSA-N
Formula: C6H5BrO
SMILES: Oc1ccccc1Br
Mol. weight [g/mol]: 173.01
CAS: 95-56-7

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
hvap	50.67	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.155		Crippen Method
mcvol	95.010	ml/mol	McGowan Method
pc	6451.51	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1043.50		NIST Webbook
rinpol	1039.00		NIST Webbook
tb	510.14	K	Joback Method
tc	761.97	K	Joback Method
tf	355.32	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.03	J/mol×K	510.14	Joback Method

cpg	183.39	J/mol×K	552.11	Joback Method
cpg	190.89	J/mol×K	594.08	Joback Method
cpg	197.65	J/mol×K	636.05	Joback Method
cpg	203.78	J/mol×K	678.02	Joback Method
cpg	209.39	J/mol×K	720.00	Joback Method
cpg	214.59	J/mol×K	761.97	Joback Method
dvisc	0.0025966	Pa×s	355.32	Joback Method
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	0.0002481	Pa×s	458.53	Joback Method
dvisc	0.0001613	Pa×s	484.34	Joback Method
dvisc	0.0001095	Pa×s	510.14	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95567&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume