Phenol, 3-bromo-

Other names: Phenol, m-bromo-
m-Bromophenol
3-Bromophenol
Inchi: InChI=1S/C6H5BrO/c7-5-2-1-3-6(8)4-5/h1-4,8H
InchiKey: MNOJRWOWILAHAV-UHFFFAOYSA-N
Formula: C6H5BrO
SMILES: Oc1cccc(Br)c1
Mol. weight [g/mol]: 173.01
CAS: 591-20-8

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	1256.10		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1256.10		NIST Webbook
rinpol	1312.00		NIST Webbook
tb	509.70	K	NIST Webbook
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
hvapt	73.50	kJ/mol	460.00	NIST Webbook

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=C591208&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
hvapt:	Enthalpy of vaporization at a given temperature
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