Benzoic acid, 2-bromo-

Other names:	2-bromobenzoic acid
	Benzoic acid, o-bromo-
	o-bromobenzoic acid
Inchi:	InChI=1S/C7H5BrO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)
InchiKey:	XRXMNWGCKISMOH-UHFFFAOYSA-N
Formula:	C7H5BrO2
SMILES:	O=C(O)c1ccccc1Br
Mol. weight [g/mol]:	201.02
CAS:	88-65-3

Physical Properties

Property code	Value	Unit	Source
chs	-3084.90 ± 4.20	kJ/mol	NIST Webbook
chs	-3100.80 ± 1.00	kJ/mol	NIST Webbook
chs	-3126.30 ± 2.10	kJ/mol	NIST Webbook
gf	-140.58	kJ/mol	Joback Method
hf	-246.90 ± 2.10	kJ/mol	NIST Webbook
hf	-257.40 ± 1.80	kJ/mol	NIST Webbook
hfs	-342.80 ± 2.10	kJ/mol	NIST Webbook
hfs	-368.30 ± 1.40	kJ/mol	NIST Webbook
hfus	24.83	kJ/mol	Thermodynamic study of the sublimation of six halobenzoic acids
hsub	108.50 ± 0.60	kJ/mol	NIST Webbook
hsub	95.90 ± 0.40	kJ/mol	NIST Webbook
hsub	110.90 ± 1.10	kJ/mol	NIST Webbook
hsub	110.90 ± 1.10	kJ/mol	NIST Webbook
hvap	63.97	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.147		Crippen Method
mcvol	110.670	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	1459.00		NIST Webbook
tb	603.43	K	Joback Method
tc	827.33	K	Joback Method
tf	421.90 ± 3.00	K	NIST Webbook
tf	420.90 ± 3.00	K	NIST Webbook
tf	421.70 ± 3.00	K	NIST Webbook

tf	419.90 ± 4.00	K	NIST Webbook
tf	419.20 ± 4.00	K	NIST Webbook
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.92	J/mol×K	603.43	Joback Method
cpg	252.43	J/mol×K	790.02	Joback Method
cpg	247.09	J/mol×K	752.70	Joback Method
cpg	241.31	J/mol×K	715.38	Joback Method
cpg	235.04	J/mol×K	678.06	Joback Method
cpg	228.26	J/mol×K	640.75	Joback Method
cpg	257.35	J/mol×K	827.33	Joback Method
cps	153.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0028538	Pa×s	378.14	Joback Method
dvisc	0.0001209	Pa×s	603.43	Joback Method
dvisc	0.0001719	Pa×s	565.88	Joback Method
dvisc	0.0002570	Pa×s	528.33	Joback Method
dvisc	0.0004086	Pa×s	490.79	Joback Method
dvisc	0.0007015	Pa×s	453.24	Joback Method
dvisc	0.0013281	Pa×s	415.69	Joback Method
hfust	24.83	kJ/mol	421.60	NIST Webbook
hsubt	106.80 ± 0.40	kJ/mol	337.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88653&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic study of the sublimation of six halobenzoic acids: https://www.doi.org/10.1016/j.jct.2004.09.005

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
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