Benzoic acid, 3-bromo-

Other names:	3-bromobenzoic acid
	Benzoic acid, m-bromo-
	m-bromobenzoic acid
Inchi:	InChI=1S/C7H5BrO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	VOIZNVUXCQLQHS-UHFFFAOYSA-N
Formula:	C7H5BrO2
SMILES:	O=C(O)c1cccc(Br)c1
Mol. weight [g/mol]:	201.02
CAS:	585-76-2

Physical Properties

Property code	Value	Unit	Source
chs	-3074.40 ± 0.80	kJ/mol	NIST Webbook
chs	-3101.60 ± 1.50	kJ/mol	NIST Webbook
gf	-140.58	kJ/mol	Joback Method
hf	-268.30 ± 1.50	kJ/mol	NIST Webbook
hf	-289.70 ± 1.60	kJ/mol	NIST Webbook
hfs	-367.50 ± 1.50	kJ/mol	NIST Webbook
hfs	-394.70 ± 1.20	kJ/mol	NIST Webbook
hfus	24.91	kJ/mol	Thermodynamic study of the sublimation of six halobenzoic acids
hsub	99.20 ± 0.20	kJ/mol	NIST Webbook
hsub	105.00 ± 1.10	kJ/mol	NIST Webbook
hsub	105.00 ± 1.10	kJ/mol	NIST Webbook
hsub	105.90 ± 0.70	kJ/mol	NIST Webbook
hvap	63.97	kJ/mol	Joback Method
ie	9.70 ± 0.20	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.147		Crippen Method
mcvol	110.670	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	1425.00		NIST Webbook
tb	553.00	K	NIST Webbook
tc	827.33	K	Joback Method
tf	428.00	K	NIST Webbook
tf	427.00 ± 4.00	K	NIST Webbook
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.35	J/mol×K	827.33	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	220.92	J/mol×K	603.43	Joback Method
cps	151.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0001209	Pa×s	603.43	Joback Method
dvisc	0.0028538	Pa×s	378.14	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	24.91	kJ/mol	430.10	NIST Webbook
hsubt	104.20 ± 0.50	kJ/mol	337.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C585762&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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