p-Bromobenzoic acid

Other names:	4-bromobenzoic acid Benzoic acid, p-bromo- benzoic acid, 4-bromo- p-Carboxybromobenzene
Inchi:	InChI=1S/C7H5BrO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	TUXYZHVUPGXXQG-UHFFFAOYSA-N
Formula:	C7H5BrO2
SMILES:	O=C(O)c1ccc(Br)cc1
Mol. weight [g/mol]:	201.02

Physical Properties

Property code	Value	Unit	Source
af	0.6594		Cheméo Relay (1.0)
chs	-3091.80 ± 1.30	kJ/mol	NIST Webbook
chs	-3089.50 ± 0.90	kJ/mol	NIST Webbook
chs	-3090.10 ± 1.30	kJ/mol	NIST Webbook
chs	-3090.80 ± 2.10	kJ/mol	NIST Webbook
gf	-140.58	kJ/mol	Joback Method
hf	-275.90 ± 1.40	kJ/mol	NIST Webbook
hf	-272.00 ± 1.70	kJ/mol	NIST Webbook
hf	-290.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-379.60 ± 1.30	kJ/mol	NIST Webbook
hfs	-379.00 ± 1.30	kJ/mol	NIST Webbook
hfs	-377.40 ± 1.60	kJ/mol	NIST Webbook
hfs	-378.00 ± 2.00	kJ/mol	NIST Webbook
hfus	30.87	kJ/mol	Thermodynamic study of the sublimation of six halobenzoic acids
hsub	103.10 ± 0.60	kJ/mol	NIST Webbook
hsub	107.60 ± 1.10	kJ/mol	NIST Webbook
hsub	87.90 ± 4.20	kJ/mol	NIST Webbook
hsub	107.60 ± 1.10	kJ/mol	NIST Webbook
hvap	94.33	kJ/mol	Cheméo Relay (1.0)
ie	9.70 ± 0.20	eV	NIST Webbook
log10ws	-2.92		Cheméo Relay (1.0)
logp	2.147		Crippen Method
mcvol	110.670	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method

rinpol	1415.00		NIST Webbook
tb	557.75	K	Cheméo Relay (1.0)
tc	804.63	K	Cheméo Relay (1.0)
tf	529.00 ± 4.00	K	NIST Webbook
tf	527.00 ± 4.00	K	NIST Webbook
tf	531.00 ± 3.00	K	NIST Webbook
vc	0.379	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.92	J/mol×K	603.43	Joback Method
cpg	228.26	J/mol×K	640.75	Joback Method
cpg	235.04	J/mol×K	678.06	Joback Method
cpg	241.31	J/mol×K	715.38	Joback Method
cpg	247.09	J/mol×K	752.70	Joback Method
cpg	252.43	J/mol×K	790.02	Joback Method
cpg	257.35	J/mol×K	827.33	Joback Method
cps	151.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0028538	Pa×s	378.14	Joback Method
dvisc	0.0013281	Pa×s	415.69	Joback Method
dvisc	0.0007015	Pa×s	453.24	Joback Method
dvisc	0.0004086	Pa×s	490.79	Joback Method
dvisc	0.0002570	Pa×s	528.33	Joback Method
dvisc	0.0001719	Pa×s	565.88	Joback Method
dvisc	0.0001209	Pa×s	603.43	Joback Method
hfust	30.87	kJ/mol	526.30	NIST Webbook
hsubt	107.40 ± 0.50	kJ/mol	357.50	NIST Webbook
hsubt	110.10 ± 0.80	kJ/mol	357.50	NIST Webbook

Sources

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

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C586765&Units=SI

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

https://www.doi.org/10.1016/j.jct.2008.11.008

Legend

af:	Acentric Factor
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