

Benzoic acid, 4-bromo-

Other names:	4-bromobenzoic acid Benzoic acid, p-bromo- p-Carboxybromobenzene p-bromobenzoic acid
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
CAS:	586-76-5

Physical Properties

Property code	Value	Unit	Source
chs	-3091.80 ± 1.30	kJ/mol	NIST Webbook
chs	-3090.80 ± 2.10	kJ/mol	NIST Webbook
chs	-3089.50 ± 0.90	kJ/mol	NIST Webbook
chs	-3090.10 ± 1.30	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	-379.00 ± 1.30	kJ/mol	NIST Webbook
hfs	-379.60 ± 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	107.60 ± 1.10	kJ/mol	NIST Webbook
hsub	87.90 ± 4.20	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

rmpol	1415.00		NIST Webbook
tb	603.43	K	Joback Method
tc	827.33	K	Joback Method
tf	527.00 ± 4.00	K	NIST Webbook
tf	531.00 ± 3.00	K	NIST Webbook
tf	529.00 ± 4.00	K	NIST Webbook
vc	0.406	m ³ /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	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
cps	151.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0001719	Paxs	565.88	Joback Method
dvisc	0.0001209	Paxs	603.43	Joback Method
dvisc	0.0028538	Paxs	378.14	Joback Method
dvisc	0.0013281	Paxs	415.69	Joback Method
dvisc	0.0007015	Paxs	453.24	Joback Method
dvisc	0.0004086	Paxs	490.79	Joback Method
dvisc	0.0002570	Paxs	528.33	Joback Method
hfust	30.87	kJ/mol	526.30	NIST Webbook
hsubt	110.10 ± 0.80	kJ/mol	357.50	NIST Webbook
hsubt	107.40 ± 0.50	kJ/mol	357.50	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Thermodynamic study of the sublimation of six halobenzoic acids: Joback Method:

<https://www.doi.org/10.1016/j.jct.2004.09.005>

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=C586765&Units=SI>

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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