

3-Bromophenylacetic acid

Other names:	Benzeneacetic acid, 3-bromo-
Inchi:	InChI=1S/C8H7BrO2/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	KYNNBXCXUOREX-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	O=C(O)Cc1cccc(Br)c1
Mol. weight [g/mol]:	215.04
CAS:	1878-67-7

Physical Properties

Property code	Value	Unit	Source
gf	-132.16	kJ/mol	Joback Method
hf	-221.87	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.076		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	626.31	K	Joback Method
tc	846.15	K	Joback Method
tf	389.41	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.66	J/molxK	626.31	Joback Method
cpg	273.99	J/molxK	662.95	Joback Method
cpg	281.72	J/molxK	699.59	Joback Method
cpg	288.89	J/molxK	736.23	Joback Method
cpg	295.54	J/molxK	772.87	Joback Method
cpg	301.71	J/molxK	809.51	Joback Method
cpg	307.42	J/molxK	846.15	Joback Method
dvisc	0.0024938	Paxs	389.41	Joback Method

dvisc	0.0011440	Paxs	428.89	Joback Method
dvisc	0.0005985	Paxs	468.38	Joback Method
dvisc	0.0003463	Paxs	507.86	Joback Method
dvisc	0.0002168	Paxs	547.34	Joback Method
dvisc	0.0001446	Paxs	586.83	Joback Method
dvisc	0.0001015	Paxs	626.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1878677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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