p-Bromophenylacetic acid

Other names:	p-Bromophenylacetic acid
	4-Bromophenylacetic acid acid
	Benzeneacetic acid, 4-bromo-
	Acetic acid, (p-bromophenyl)-
Inchi:	InChI=1S/C8H7BrO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	QOWSWEBLNVACCL-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	O=C(O)Cc1ccc(Br)cc1
Mol. weight [g/mol]:	215.05

Physical Properties

Property code	Value	Unit	Source
hf	-298.30	kJ/mol	Cheméo Relay (1.0)
hfus	21.10	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.076		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	569.26	K	Cheméo Relay (1.0)
tf	412.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.66	J/mol×K	626.31	Joback Method
cpg	307.42	J/mol×K	846.15	Joback Method
cpg	301.71	J/mol×K	809.51	Joback Method
cpg	295.54	J/mol×K	772.87	Joback Method
cpg	288.89	J/mol×K	736.23	Joback Method
cpg	281.72	J/mol×K	699.59	Joback Method
cpg	273.99	J/mol×K	662.95	Joback Method
dvisc	0.0003463	Pa×s	507.86	Joback Method

dvisc	0.0001015	Pa×s	626.31	Joback Method
dvisc	0.0001446	Pa×s	586.83	Joback Method
dvisc	0.0002168	Pa×s	547.34	Joback Method
dvisc	0.0024938	Pa×s	389.41	Joback Method
dvisc	0.0005985	Pa×s	468.38	Joback Method
dvisc	0.0011440	Pa×s	428.89	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1878688&Units=SI

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

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

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

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point