.alpha.-Bromophenyl acetic acid

Other names: dl-«alpha»-Bromophenylacetic acid
Benzeneacetic acid, «alpha»-bromo-
bromo(phenyl)acetic acid
Inchi: InChI=1S/C8H7BrO2/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H,(H,10,11)
InchiKey: WAKFRZBXTKUFIW-UHFFFAOYSA-N
Formula: C8H7BrO2
SMILES: O=C(O)C(Br)c1ccccc1
Mol. weight [g/mol]: 215.05

Physical Properties

Property code	Value	Unit	Source
hf	-295.49	kJ/mol	Cheméo Relay (1.0)
hfus	17.97	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-1.55		Cheméo Relay (1.0)
logp	2.207		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
tb	555.02	K	Cheméo Relay (1.0)
tf	383.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.76	J/mol×K	620.89	Joback Method
cpg	276.52	J/mol×K	658.13	Joback Method
cpg	284.60	J/mol×K	695.37	Joback Method
cpg	292.04	J/mol×K	732.62	Joback Method
cpg	298.89	J/mol×K	769.86	Joback Method
cpg	305.19	J/mol×K	807.10	Joback Method
cpg	311.00	J/mol×K	844.34	Joback Method
dvisc	0.0048342	Pa×s	361.89	Joback Method
dvisc	0.0017838	Pa×s	405.06	Joback Method
dvisc	0.0007976	Pa×s	448.22	Joback Method

dvisc	0.0004108	Pa×s	491.39	Joback Method
dvisc	0.0002355	Pa×s	534.56	Joback Method
dvisc	0.0001467	Pa×s	577.72	Joback Method
dvisc	0.0000976	Pa×s	620.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4870659&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point