«alpha»-Bromophenylacetic 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]: 215.04
CAS: 4870-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-124.97	kJ/mol	Joback Method
hf	-215.68	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.207		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
tb	620.89	K	Joback Method
tc	844.34	K	Joback Method
tf	361.89	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.76	J/mol×K	620.89	Joback Method
cpg	305.19	J/mol×K	807.10	Joback Method
cpg	298.89	J/mol×K	769.86	Joback Method
cpg	292.04	J/mol×K	732.62	Joback Method
cpg	284.60	J/mol×K	695.37	Joback Method
cpg	276.52	J/mol×K	658.13	Joback Method

cpg	311.00	J/mol×K	844.34	Joback Method
dvisc	0.0000976	Pa×s	620.89	Joback Method
dvisc	0.0001467	Pa×s	577.72	Joback Method
dvisc	0.0002355	Pa×s	534.56	Joback Method
dvisc	0.0004108	Pa×s	491.39	Joback Method
dvisc	0.0007976	Pa×s	448.22	Joback Method
dvisc	0.0017838	Pa×s	405.06	Joback Method
dvisc	0.0048342	Pa×s	361.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4870659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume