2-(4-Bromophenyl)propionic acid

Other names: Benzeneacetic acid, 4-bromo-«alpha»-methyl-
2-(4-Bromophenyl)propanoic acid
Inchi: InChI=1S/C9H9BrO2/c1-6(9(11)12)7-2-4-8(10)5-3-7/h2-6H,1H3,(H,11,12)
InchiKey: PFDBEACWLCHWRZ-UHFFFAOYSA-N
Formula: C9H9BrO2
SMILES: CC(C(=O)O)c1ccc(Br)cc1
Mol. weight [g/mol]: 229.07
CAS: 53086-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-126.18	kJ/mol	Joback Method
hf	-247.79	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	68.04	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.637		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	1574.00		NIST Webbook
tb	648.75	K	Joback Method
tc	869.08	K	Joback Method
tf	385.68	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.58	J/mol×K	648.75	Joback Method
cpg	322.00	J/mol×K	685.47	Joback Method
cpg	330.75	J/mol×K	722.19	Joback Method
cpg	338.88	J/mol×K	758.92	Joback Method
cpg	346.41	J/mol×K	795.64	Joback Method
cpg	353.40	J/mol×K	832.36	Joback Method

cpg	359.87	J/mol×K	869.08	Joback Method
dvisc	0.0029098	Pa×s	385.68	Joback Method
dvisc	0.0011743	Pa×s	429.52	Joback Method
dvisc	0.0005607	Pa×s	473.37	Joback Method
dvisc	0.0003034	Pa×s	517.22	Joback Method
dvisc	0.0001808	Pa×s	561.06	Joback Method
dvisc	0.0001161	Pa×s	604.90	Joback Method
dvisc	0.0000791	Pa×s	648.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53086536&Units=SI

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
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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