

3-Bromo-4-methoxyphenylacetic acid

Inchi:	InChI=1S/C9H9BrO3/c1-13-8-3-2-6(4-7(8)10)5-9(11)12/h2-4H,5H2,1H3,(H,11,12)
InchiKey:	POTVGQUUEQTPNA-UHFFFAOYSA-N
Formula:	C9H9BrO3
SMILES:	COc1ccc(CC(=O)O)cc1Br
Mol. weight [g/mol]:	245.07
CAS:	774-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-238.37	kJ/mol	Joback Method
hf	-386.20	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.085		Crippen Method
mcvol	144.720	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	676.59	K	Joback Method
tc	891.07	K	Joback Method
tf	435.43	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.69	J/molxK	676.59	Joback Method
cpg	341.68	J/molxK	712.34	Joback Method
cpg	350.09	J/molxK	748.08	Joback Method
cpg	357.94	J/molxK	783.83	Joback Method
cpg	365.25	J/molxK	819.58	Joback Method
cpg	372.02	J/molxK	855.32	Joback Method
cpg	378.28	J/molxK	891.07	Joback Method
dvisc	0.0010385	Paxs	435.43	Joback Method
dvisc	0.0005305	Paxs	475.62	Joback Method

dvisc	0.0003009	Paxs	515.82	Joback Method
dvisc	0.0001852	Paxs	556.01	Joback Method
dvisc	0.0001217	Paxs	596.20	Joback Method
dvisc	0.0000844	Paxs	636.40	Joback Method
dvisc	0.0000611	Paxs	676.59	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C774812&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
mccvol:	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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