2-Bromo-3-methoxybenzoic acid

Inchi: InChI=1S/C8H7BrO3/c1-12-6-4-2-3-5(7(6)9)8(10)11/h2-4H,1H3,(H,10,11)
InchiKey: AOGGEUOQUYCZAH-UHFFFAOYSA-N
Formula: C8H7BrO3
SMILES: COc1cccc(C(=O)O)c1Br
Mol. weight [g/mol]: 231.04
CAS: 88377-29-1

Physical Properties

Property code	Value	Unit	Source
gf	-246.79	kJ/mol	Joback Method
hf	-365.56	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.156		Crippen Method
mcvol	130.630	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
tb	653.71	K	Joback Method
tc	871.75	K	Joback Method
tf	424.16	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.36	J/mol×K	653.71	Joback Method
cpg	293.49	J/mol×K	690.05	Joback Method
cpg	301.10	J/mol×K	726.39	Joback Method
cpg	308.19	J/mol×K	762.73	Joback Method
cpg	314.78	J/mol×K	799.07	Joback Method
cpg	320.89	J/mol×K	835.41	Joback Method
cpg	326.51	J/mol×K	871.75	Joback Method
dvisc	0.0011818	Pa×s	424.16	Joback Method
dvisc	0.0006128	Pa×s	462.42	Joback Method

dvisc	0.0003513	Pa×s	500.68	Joback Method
dvisc	0.0002179	Pa×s	538.94	Joback Method
dvisc	0.0001440	Pa×s	577.19	Joback Method
dvisc	0.0001002	Pa×s	615.45	Joback Method
dvisc	0.0000728	Pa×s	653.71	Joback Method

Sources

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=C88377291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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