

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/molxK	653.71	Joback Method
cpg	293.49	J/molxK	690.05	Joback Method
cpg	301.10	J/molxK	726.39	Joback Method
cpg	308.19	J/molxK	762.73	Joback Method
cpg	314.78	J/molxK	799.07	Joback Method
cpg	320.89	J/molxK	835.41	Joback Method
cpg	326.51	J/molxK	871.75	Joback Method
dvisc	0.0011818	Paxs	424.16	Joback Method
dvisc	0.0006128	Paxs	462.42	Joback Method

dvisc	0.0003513	Paxs	500.68	Joback Method
dvisc	0.0002179	Paxs	538.94	Joback Method
dvisc	0.0001440	Paxs	577.19	Joback Method
dvisc	0.0001002	Paxs	615.45	Joback Method
dvisc	0.0000728	Paxs	653.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88377291&Units=SI
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

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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