2-Bromo-5-fluorobenzoic acid, methyl ester

Other names: Benzoic acid, 2-bromo-5-fluoro-, methyl ester
methyl 2-bromo-5-fluorobenzoate
Inchi: InChI=1S/C8H6BrFO2/c1-12-8(11)6-4-5(10)2-3-7(6)9/h2-4H,1H3
InchiKey: FCMQMRAFVRTHCR-UHFFFAOYSA-N
Formula: C8H6BrFO2
SMILES: COC(=O)c1cc(F)ccc1Br
Mol. weight [g/mol]: 233.03
CAS: 6942-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-304.78	kJ/mol	Joback Method
hf	-409.44	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.375		Crippen Method
mcvol	126.530	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	560.80	K	Joback Method
tc	786.19	K	Joback Method
tf	363.93	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.13	J/mol×K	560.80	Joback Method
cpg	263.58	J/mol×K	598.36	Joback Method
cpg	272.46	J/mol×K	635.93	Joback Method
cpg	280.77	J/mol×K	673.49	Joback Method
cpg	288.54	J/mol×K	711.06	Joback Method
cpg	295.76	J/mol×K	748.62	Joback Method
cpg	302.46	J/mol×K	786.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6942398&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

Legend

cpg:	Ideal gas heat capacity
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