m-Methoxybenzoic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C14H10BrFO3/c1-18-11-4-2-3-9(7-11)14(17)19-13-6-5-10(16)8-12(13)15/h2-8
InchiKey: DJTKDHRPVWRPQY-UHFFFAOYSA-N
Formula: C14H10BrFO3
SMILES: COc1cccc(C(=O)Oc2ccc(F)cc2Br)c1
Mol. weight [g/mol]: 325.13

Physical Properties

Property code	Value	Unit	Source
gf	-256.48	kJ/mol	Joback Method
hf	-440.44	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	70.48	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.816		Crippen Method
mcvol	193.180	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1967.20		NIST Webbook
rinpol	1967.20		NIST Webbook
tb	752.16	K	Joback Method
tc	992.93	K	Joback Method
tf	492.72	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.69	J/mol×K	752.16	Joback Method
cpg	491.66	J/mol×K	792.29	Joback Method
cpg	502.60	J/mol×K	832.42	Joback Method
cpg	512.53	J/mol×K	872.55	Joback Method
cpg	521.47	J/mol×K	912.67	Joback Method
cpg	529.44	J/mol×K	952.80	Joback Method
cpg	536.45	J/mol×K	992.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292630&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume