

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

Inchi:	InChI=1S/C14H10BrFO3/c1-18-12-5-3-2-4-10(12)14(17)19-13-7-6-9(16)8-11(13)15/h2-8
InchiKey:	IRGWJWHJODMPEF-UHFFFAOYSA-N
Formula:	C14H10BrFO3
SMILES:	COc1ccccc1C(=O)Oc1ccc(F)cc1Br
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	1960.40		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/molxK	752.16	Joback Method
cpg	491.66	J/molxK	792.29	Joback Method
cpg	502.60	J/molxK	832.42	Joback Method
cpg	512.53	J/molxK	872.55	Joback Method
cpg	521.47	J/molxK	912.67	Joback Method
cpg	529.44	J/molxK	952.80	Joback Method
cpg	536.45	J/molxK	992.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292618&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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