Phenylacetic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C14H10BrFO2/c15-12-9-11(16)6-7-13(12)18-14(17)8-10-4-2-1-3-5-10/h1-7,9H

InchiKey: XMLJZNPMOWWODA-UHFFFAOYSA-N

Formula: C14H10BrFO2

SMILES: O=C(Cc1ccccc1)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 309.13

Physical Properties

Property code	Value	Unit	Source
gf	-141.85	kJ/mol	Joback Method
hf	-296.75	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.736		Crippen Method
mcvol	187.310	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	724.76	K	Joback Method
tc	968.45	K	Joback Method
tf	457.97	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.84	J/mol×K	724.76	Joback Method
cpg	469.28	J/mol×K	765.37	Joback Method
cpg	480.66	J/mol×K	805.99	Joback Method
cpg	491.04	J/mol×K	846.60	Joback Method
cpg	500.48	J/mol×K	887.22	Joback Method
cpg	509.01	J/mol×K	927.83	Joback Method
cpg	516.70	J/mol×K	968.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299006&Units=SI

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