3-Bromobenzoic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C13H7Br2FO2/c14-9-3-1-2-8(6-9)13(17)18-12-5-4-10(16)7-11(12)15/h1-7H
InchiKey: MNLMCXWAMPPDIB-UHFFFAOYSA-N
Formula: C13H7Br2FO2
SMILES: O=C(Oc1ccc(F)cc1Br)c1cccc(Br)c1
Mol. weight [g/mol]: 374.00

Physical Properties

Property code	Value	Unit	Source
gf	-145.58	kJ/mol	Joback Method
hf	-261.25	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.570		Crippen Method
mcvol	190.720	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	2152.50		NIST Webbook
tb	773.02	K	Joback Method
tc	1032.58	K	Joback Method
tf	519.02	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.65	J/mol×K	773.02	Joback Method
cpg	443.73	J/mol×K	816.28	Joback Method
cpg	452.84	J/mol×K	859.54	Joback Method
cpg	461.05	J/mol×K	902.80	Joback Method
cpg	468.44	J/mol×K	946.06	Joback Method
cpg	475.05	J/mol×K	989.32	Joback Method
cpg	480.95	J/mol×K	1032.58	Joback Method

Sources

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=U292666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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