2,6-Difluorobenzoic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C13H6BrF3O2/c14-8-6-7(15)4-5-11(8)19-13(18)12-9(16)2-1-3-10(12)17/h1-6H

InchiKey: QNQIJILNZGYDQY-UHFFFAOYSA-N

Formula: C13H6BrF3O2

SMILES: O=C(Oc1ccc(F)cc1Br)c1c(F)cccc1F

Mol. weight [g/mol]: 331.08

Physical Properties

Property code	Value	Unit	Source
gf	-559.15	kJ/mol	Joback Method
hf	-691.27	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.086		Crippen Method
mcvol	176.760	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1822.30		NIST Webbook
tb	710.38	K	Joback Method
tc	939.36	K	Joback Method
tf	472.92	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.07	J/mol×K	710.38	Joback Method
cpg	429.47	J/mol×K	748.54	Joback Method
cpg	439.05	J/mol×K	786.71	Joback Method
cpg	447.83	J/mol×K	824.87	Joback Method
cpg	455.83	J/mol×K	863.03	Joback Method
cpg	463.09	J/mol×K	901.19	Joback Method
cpg	469.62	J/mol×K	939.36	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=U292625&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