3-Bromobenzoic acid, 5-fluoro-2-nitrophenyl ester

Inchi: InChI=1S/C13H7BrFNO4/c14-9-3-1-2-8(6-9)13(17)20-12-7-10(15)4-5-11(12)16(18)19/h1

InchiKey: SWPIYHGPBHSHRR-UHFFFAOYSA-N

Formula: C13H7BrFNO4

SMILES: O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1cccc(Br)c1

Mol. weight [g/mol]: 340.10

Physical Properties

Property code	Value	Unit	Source
gf	-124.35	kJ/mol	Joback Method
hf	-298.34	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	3.716		Crippen Method
mcvol	190.640	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	2247.80		NIST Webbook
rinpol	2247.80		NIST Webbook
tb	858.70	K	Joback Method
tc	1124.57	K	Joback Method
tf	602.83	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.27	J/mol×K	858.70	Joback Method
cpg	497.38	J/mol×K	903.01	Joback Method
cpg	505.44	J/mol×K	947.32	Joback Method
cpg	512.50	J/mol×K	991.63	Joback Method
cpg	518.63	J/mol×K	1035.94	Joback Method
cpg	523.89	J/mol×K	1080.25	Joback Method
cpg	528.33	J/mol×K	1124.57	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=U292668&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