Benzoic acid, (2-fluoro-5-nitrophenyl)methyl ester

Inchi: InChI=1S/C14H10FNO4/c15-13-7-6-12(16(18)19)8-11(13)9-20-14(17)10-4-2-1-3-5-10/h1

InchiKey: WTPUBICIJXMFPS-UHFFFAOYSA-N

Formula: C14H10FNO4

SMILES: O=C(OCc1cc([N+](=O)[O-])ccc1F)c1ccccc1

Mol. weight [g/mol]: 275.23

Physical Properties

Property code	Value	Unit	Source
gf	-120.62	kJ/mol	Joback Method
hf	-333.84	kJ/mol	Joback Method
hfus	36.55	kJ/mol	Joback Method
hvap	77.56	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.091		Crippen Method
mcvol	187.230	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	2207.00		NIST Webbook
tb	810.44	K	Joback Method
tc	1061.68	K	Joback Method
tf	541.78	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.51	J/mol×K	810.44	Joback Method
cpg	527.92	J/mol×K	852.31	Joback Method
cpg	538.17	J/mol×K	894.19	Joback Method
cpg	547.32	J/mol×K	936.06	Joback Method
cpg	555.43	J/mol×K	977.94	Joback Method
cpg	562.53	J/mol×K	1019.81	Joback Method
cpg	568.69	J/mol×K	1061.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368239&Units=SI
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

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