Isophthalic acid, monoamide, N-(2-fluorophenyl)-, ethyl ester

Inchi: InChI=1S/C16H14FNO3/c1-2-21-16(20)12-7-5-6-11(10-12)15(19)18-14-9-4-3-8-13(14)17

InchiKey: WIGWYQSJFXWMOC-UHFFFAOYSA-N

Formula: C16H14FNO3

SMILES: CCOC(=O)c1cccc(C(O)=Nc2ccccc2F)c1

Mol. weight [g/mol]: 287.29

Physical Properties

Property code	Value	Unit	Source
hf	-444.16	kJ/mol	Joback Method
hvap	85.50	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.639		Crippen Method
mcvol	209.540	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	873.10	K	Joback Method
tc	1098.99	K	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=U345774&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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