Isophthalic acid, diamide N,N'-di(2-fluorophenyl)-

Inchi: InChI=1S/C20H14F2N2O2/c21-15-8-1-3-10-17(15)23-19(25)13-6-5-7-14(12-13)20(26)24-18-11-4-2-9-16(18)22/h1-12H,(H,23,25)(H,24,26)

InchiKey: NGMBMIKWVLIQJO-UHFFFAOYSA-N

Formula: C20H14F2N2O2

SMILES: OC(=Nc1ccccc1F)c1cccc(C(O)=Nc2ccccc2F)c1

Mol. weight [g/mol]: 352.33

Physical Properties

Property code	Value	Unit	Source
hf	-332.77	kJ/mol	Joback Method
hvap	107.44	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.237		Crippen Method
mcvol	248.020	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook
tb	1088.00	K	Joback Method
tc	1336.70	K	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=U345784&Units=SI

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