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

Inchi: InChI=1S/C18H18FNO3/c1-12(2)11-23-18(22)14-7-5-6-13(10-14)17(21)20-16-9-4-3-8-15

InchiKey: QHCNAYWMFFUCTI-UHFFFAOYSA-N

Formula: C18H18FNO3

SMILES: CC(C)COC(=O)c1cccc(C(=O)Nc2ccccc2F)c1

Mol. weight [g/mol]: 315.34

Physical Properties

Property code	Value	Unit	Source
gf	-164.46	kJ/mol	Joback Method
hf	-470.03	kJ/mol	Joback Method
hfus	38.72	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	3.891		Crippen Method
mcvol	237.720	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2569.00		NIST Webbook
rinpol	2569.00		NIST Webbook
tb	853.72	K	Joback Method
tc	1080.24	K	Joback Method
tf	530.84	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.74	J/mol×K	853.72	Joback Method
cpg	714.77	J/mol×K	891.47	Joback Method
cpg	726.63	J/mol×K	929.23	Joback Method
cpg	737.37	J/mol×K	966.98	Joback Method
cpg	747.03	J/mol×K	1004.74	Joback Method
cpg	755.66	J/mol×K	1042.49	Joback Method
cpg	763.31	J/mol×K	1080.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345776&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

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