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

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

InchiKey: HNAIWKRNFFUCJY-UHFFFAOYSA-N

Formula: C18H18FNO3

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

Mol. weight [g/mol]: 315.34

Physical Properties

Property code	Value	Unit	Source
gf	-162.02	kJ/mol	Joback Method
hf	-464.75	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	83.06	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.035		Crippen Method
mcvol	237.720	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2652.00		NIST Webbook
rinpol	2652.00		NIST Webbook
tb	854.16	K	Joback Method
tc	1077.63	K	Joback Method
tf	545.84	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.17	J/mol×K	854.16	Joback Method
cpg	714.05	J/mol×K	891.41	Joback Method
cpg	725.80	J/mol×K	928.65	Joback Method
cpg	736.47	J/mol×K	965.90	Joback Method
cpg	746.11	J/mol×K	1003.14	Joback Method
cpg	754.75	J/mol×K	1040.39	Joback Method
cpg	762.45	J/mol×K	1077.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345777&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