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

Inchi: InChI=1S/C19H20FNO3/c1-2-3-6-12-24-19(23)15-9-7-8-14(13-15)18(22)21-17-11-5-4-10

InchiKey: CFORUZMHLFSHTN-UHFFFAOYSA-N

Formula: C19H20FNO3

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

Mol. weight [g/mol]: 329.37

Physical Properties

Property code	Value	Unit	Source
gf	-153.60	kJ/mol	Joback Method
hf	-485.39	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	85.28	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.425		Crippen Method
mcvol	251.810	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook
tb	877.04	K	Joback Method
tc	1098.85	K	Joback Method
tf	557.11	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.81	J/mol×K	877.04	Joback Method
cpg	770.88	J/mol×K	914.01	Joback Method
cpg	782.80	J/mol×K	950.98	Joback Method
cpg	793.62	J/mol×K	987.94	Joback Method
cpg	803.40	J/mol×K	1024.91	Joback Method
cpg	812.19	J/mol×K	1061.88	Joback Method
cpg	820.02	J/mol×K	1098.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345778&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