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

Inchi: InChI=1S/C20H22FNO3/c1-2-3-4-7-13-25-20(24)16-10-8-9-15(14-16)19(23)22-18-12-6-5

InchiKey: MBSOULYUNCVAOQ-UHFFFAOYSA-N

Formula: C20H22FNO3

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

Mol. weight [g/mol]: 343.39

Physical Properties

Property code	Value	Unit	Source
gf	-145.18	kJ/mol	Joback Method
hf	-506.03	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	87.51	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.815		Crippen Method
mcvol	265.900	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	899.92	K	Joback Method
tc	1120.76	K	Joback Method
tf	568.38	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.24	J/mol×K	899.92	Joback Method
cpg	828.46	J/mol×K	936.73	Joback Method
cpg	840.53	J/mol×K	973.53	Joback Method
cpg	851.48	J/mol×K	1010.34	Joback Method
cpg	861.39	J/mol×K	1047.15	Joback Method
cpg	870.28	J/mol×K	1083.96	Joback Method
cpg	878.22	J/mol×K	1120.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345780&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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