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

Inchi: InChI=1S/C22H26FNO3/c1-2-3-4-5-6-9-15-27-22(26)18-12-10-11-17(16-18)21(25)24-20-

InchiKey: SMRQBPBPYCEKKW-UHFFFAOYSA-N

Formula: C22H26FNO3

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

Mol. weight [g/mol]: 371.45

Physical Properties

Property code	Value	Unit	Source
gf	-128.34	kJ/mol	Joback Method
hf	-547.31	kJ/mol	Joback Method
hfus	52.61	kJ/mol	Joback Method
hvap	91.96	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.595		Crippen Method
mcvol	294.080	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	3085.00		NIST Webbook
tb	945.68	K	Joback Method
tc	1166.90	K	Joback Method
tf	590.92	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.19	J/mol×K	945.68	Joback Method
cpg	945.72	J/mol×K	982.55	Joback Method
cpg	958.04	J/mol×K	1019.42	Joback Method
cpg	969.22	J/mol×K	1056.29	Joback Method
cpg	979.31	J/mol×K	1093.16	Joback Method
cpg	988.37	J/mol×K	1130.03	Joback Method
cpg	996.46	J/mol×K	1166.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345782&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