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

Inchi: InChI=1S/C20H22FNO3/c1-14(2)7-6-12-25-20(24)16-9-5-8-15(13-16)19(23)22-18-11-4-3

InchiKey: FEGDEEOBEYJBPV-UHFFFAOYSA-N

Formula: C20H22FNO3

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

Mol. weight [g/mol]: 343.39

Physical Properties

Property code	Value	Unit	Source
gf	-147.62	kJ/mol	Joback Method
hf	-511.31	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.671		Crippen Method
mcvol	265.900	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	899.48	K	Joback Method
tc	1122.69	K	Joback Method
tf	553.38	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.76	J/mol×K	899.48	Joback Method
cpg	829.09	J/mol×K	936.68	Joback Method
cpg	841.22	J/mol×K	973.88	Joback Method
cpg	852.21	J/mol×K	1011.09	Joback Method
cpg	862.11	J/mol×K	1048.29	Joback Method
cpg	870.96	J/mol×K	1085.49	Joback Method
cpg	878.83	J/mol×K	1122.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345779&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