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

Inchi: InChI=1S/C17H16FNO3/c1-2-10-22-17(21)13-7-5-6-12(11-13)16(20)19-15-9-4-3-8-14(15

InchiKey: UBGQAJWLFAPTCI-UHFFFAOYSA-N

Formula: C17H16FNO3

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

Mol. weight [g/mol]: 301.31

Physical Properties

Property code	Value	Unit	Source
gf	-170.44	kJ/mol	Joback Method
hf	-444.11	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	80.83	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.645		Crippen Method
mcvol	223.630	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	831.28	K	Joback Method
tc	1057.08	K	Joback Method
tf	534.57	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.38	J/mol×K	831.28	Joback Method
cpg	658.04	J/mol×K	868.91	Joback Method
cpg	669.59	J/mol×K	906.55	Joback Method
cpg	680.07	J/mol×K	944.18	Joback Method
cpg	689.53	J/mol×K	981.81	Joback Method
cpg	698.00	J/mol×K	1019.45	Joback Method
cpg	705.54	J/mol×K	1057.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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