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

Inchi: InChI=1S/C19H20ClNO3/c1-2-3-6-12-24-19(23)15-9-7-8-14(13-15)18(22)21-17-11-5-4-1

InchiKey: KKFSEOBLEPTCEJ-UHFFFAOYSA-N

Formula: C19H20ClNO3

SMILES: CCCCCOC(=O)c1cccc(C(O)=Nc2ccccc2Cl)c1

Mol. weight [g/mol]: 345.82

Physical Properties

Property code	Value	Unit	Source
hf	-325.71	kJ/mol	Joback Method
hvap	97.38	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.323		Crippen Method
mcvol	262.280	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2939.00		NIST Webbook
rinpol	2939.00		NIST Webbook
tb	979.90	K	Joback Method
tc	1212.62	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345818&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

hf: Enthalpy of formation 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