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

Inchi: InChI=1S/C21H24ClNO3/c1-2-3-4-5-8-14-26-21(25)17-11-9-10-16(15-17)20(24)23-19-13

InchiKey: KEACAALLMUEHQX-UHFFFAOYSA-N

Formula: C21H24ClNO3

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

Mol. weight [g/mol]: 373.87

Physical Properties

Property code	Value	Unit	Source
hf	-366.99	kJ/mol	Joback Method
hvap	101.83	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.103		Crippen Method
mcvol	290.460	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook
tb	1025.66	K	Joback Method
tc	1260.47	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345821&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

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