

Pyridin-3-yl 3-chlorobenzoate

Inchi:	InChI=1S/C12H8ClNO2/c13-10-4-1-3-9(7-10)12(15)16-11-5-2-6-14-8-11/h1-8H
InchiKey:	DKJMMRRCBINSFH-UHFFFAOYSA-N
Formula:	C12H8ClNO2
SMILES:	O=C(Oc1ccnc1)c1cccc(Cl)c1
Mol. weight [g/mol]:	233.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.954		Crippen Method
mcvol	162.080	ml/mol	McGowan Method
rinpol	1925.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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