

N-(p-Chlorophenyl)-4-cyclohexene-1,2-dicarboxamide

Inchi:	InChI=1S/C14H12ClNO2/c15-9-5-7-10(8-6-9)16-13(17)11-3-1-2-4-12(11)14(16)18/h1-2,5
InchiKey:	LVBNTQRVWHUJOP-UHFFFAOYSA-N
Formula:	C14H12ClNO2
SMILES:	O=C1C2CC=CCC2C(=O)N1c1ccc(Cl)cc1
Mol. weight [g/mol]:	261.70
CAS:	43069-64-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.796		Crippen Method
mcvol	183.700	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43069643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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