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

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]: 261.71

Physical Properties

Property code	Value	Unit	Source
logp	2.796		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
tf	472.78	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C43069643&Units=SI

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point