

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

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/ci990307I>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/124-652-0/N-p-Chlorophenyl-4-cyclohexene-1-2-dicarboximide.pdf>

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