2-Furamidoxime, o-(p-chlorobenzoyl)-5-nitro

Inchi: InChI=1S/C12H8ClN3O5/c13-8-3-1-7(2-4-8)12(17)21-15-11(14)9-5-6-10(20-9)16(18)19/h
InchiKey: IQLCVWYUDLVGCG-UHFFFAOYSA-N
Formula: C12H8ClN3O5
SMILES: NC(=NOC(=O)c1ccc(Cl)cc1)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]: 309.66
CAS: 37784-51-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.58		Crippen Method
logp	2.318		Crippen Method
mcvol	195.350	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37784513&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

Latest version available from:
https://www.chemeo.com/cid/124-600-7/2-Furamidoxime-o-p-chlorobenzoyl-5-nitro.pdf
Generated by Cheméo on 2024-05-03 20:49:32.219116561 +0000 UTC m=+17058621.139693876.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.