

Glutarimide, N-(5-chloro-2-methoxyphenyl)-

Inchi: InChI=1S/C12H12ClNO3/c1-17-10-6-5-8(13)7-9(10)14-11(15)3-2-4-12(14)16/h5-7H,2-4H
InchiKey: RSFWOFAQOSHNTU-UHFFFAOYSA-N
Formula: C12H12ClNO3
SMILES: COc1ccc(Cl)cc1N1C(=O)CCCC1=O
Mol. weight [g/mol]: 253.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.392		Crippen Method
mcvol	176.550	ml/mol	McGowan Method
rinpole	2309.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360762&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/66-389-8/Glutarimide-N-5-chloro-2-methoxyphenyl.pdf>

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