

Glutarimide, N-(3-methylphenyl)-

Inchi: InChI=1S/C12H13NO2/c1-9-4-2-5-10(8-9)13-11(14)6-3-7-12(13)15/h2,4-5,8H,3,6-7H2,1H
InchiKey: HCNIWAWFXPZHII-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: Cc1cccc(N2C(=O)CCCC2=O)c1
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	2.039		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
rinpola	2127.00		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=U360926&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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/46-378-2/Glutarimide-N-3-methylphenyl.pdf>

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