

Chlormezanone

Other names:

4H-1,3-Thiazin-4-one, 2-(4-chlorophenyl)tetrahydro-3-methyl-, 1,1-dioxide
4H-1,3-Thiazin-4-one, 2-(p-chlorophenyl)tetrahydro-3-methyl-, 1,1-dioxide
Chlormethazanone
Chlormethazone
Chlormezanon
Fenarol
Mio-Sed
Muskel-Trancopal
Phenarol
Rilansyl
Rilaquil
Rilassol
Tanafol
Trancopal
Alinam
Banabin
Banabin-Sintyal
Bisina
Chlomedinon
Clorilax
Clormetazanone
Clormetazon
Lobak
Miorilax
Muskel
Myolespen
Rexan
Rilax
Rillasol
Supotran
Suprotan
Trancote
2-(p-Chlorophenyl)tetrahydro-3-methyl-4H-1,3-thiazin-4-one 1,1-dioxide
2-(p-Chlorophenyl)-3-methyl-1,3-perhydrothiazin-4-one, 1,1-dioxide
2-(4-Chlorophenyl)-3-methyl-4-metathiazanone-1,1-dioxide
4H-1,3-Thiazin-4-one, tetrahydro-2-(p-chlorophenyl)-3-methyl-, 1,1-dioxide
WIN 4692
Banabil-sintyal
Dichloromezanone
Rillasol

Inchi: Transanate
 (.+/-)-Chlormezanone
 (.+/-)-Fenarol
 dl-Chlormezanone
InchiKey: WEQAYVWKMWHEJO-UHFFFAOYSA-N
Formula: C11H12ClNO3S
SMILES: CN1C(=O)CCS(=O)(=O)C1c1ccc(Cl)cc1
Mol. weight [g/mol]: 273.74
CAS: 80-77-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.615		Crippen Method
mcvol	183.110	ml/mol	McGowan Method
rinpol	2194.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2150.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C80773&Units=SI>

Legend

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

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