Trimethadione

Other names:

2,4-Oxazolidinedione, 3,5,5-trimethyl-
Absentol
Edion
Epidione
Epixal
Mino aleviatin
Petidion
Petidon
Petilep
Pitmal
Ptimal
Tridion
Tridione
Tridone
Trimedal
Trimetadione
Trimethadion
Trimethin
Trimetin
Trioxanona
Troxidone
3,3,5-Trimethyl-2,4-diketooxazolidine
3,5,5-Trimethyl-2,4-oxazolidinedione
3,5,5-Trimethyloxazolidine-2,4-dione
A 2297
Absetil
Convenixa
Convexina
Epidone
Etydion
Minoaleuiatin
Petimalin
Tioxanona
Tredione
Tricione
Tridilona
Trilidona
Trimedone
Trimethdione
Triozanona

	Tromedone
	3,5,5-Trojmetylooksazolidyno-2,4-dion
	NSC 15799
	Neo-absentol
	3,5,5-Trimethyl-2,4-oxazolidinedionenol
	3,5,5-Trimethyl-1,3-oxazolidine-2,4-dione
Inchi:	InChI=1S/C6H9NO3/c1-6(2)4(8)7(3)5(9)10-6/h1-3H3
InchiKey:	IRYJRGCIQBGHIV-UHFFFAOYSA-N
Formula:	C6H9NO3
SMILES:	CN1C(=O)OC(C)(C)C1=O
Mol. weight [g/mol]:	143.14
CAS:	127-48-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.53		Crippen Method
logp	0.374		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
rinpol	1080.00		NIST Webbook
rinpol	1032.70		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1032.70		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127480&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