Methsuximide

Other names:	2,5-Pyrrolidinedione, 1,3-dimethyl-3-phenyl-
	Succinimide, N,2-dimethyl-2-phenyl-
	Celontin
	Mesuximide
	Mesuximidum
	Methsuximid
	N,2-Dimethyl-2-phenylsuccinimide
	Petinutin
	PM 396
	1,3-Dimethyl-3-phenyl-2,5-dioxopyrrolidine
	1,3-Dimethyl-3-phenyl-pyrrolidin-2,5-dione
	N-Methyl-«alpha»-methyl-«alpha»-phenylsuccinimide
	N-Methyl-«alpha»,«alpha»-methylphenylsuccinimide
	«alpha»-Methylphensuximide
	«alpha»-Methyl-«alpha»-phenyl N-methyl succinimide
	Metsuccimide
	1,3-Dimethyl-3-phenylsuccinimide
Inchi:	InChI=1S/C12H13NO2/c1-12(9-6-4-3-5-7-9)8-10(14)13(2)11(12)15/h3-7H,8H2,1-2H3
InchiKey:	AJXPJJZHWIXJCJ-UHFFFAOYSA-N
Formula:	C12H13NO2
SMILES:	CN1C(=O)CC(C)(c2ccccc2)C1=O
Mol. weight [g/mol]:	203.24
CAS:	77-41-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.333		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1599.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77418&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
rinpol:	Non-polar retention indices