

Ethotoin

Other names:	2,4-Imidazolidinedione, 3-ethyl-5-phenyl-Hydantoin, 3-ethyl-5-phenyl-Accenon AC-695 Peganone 3-Ethyl-5-phenylhydantoin 1-Ethyl-2,5-dioxo-4-phenylimidazolidine 3-Ethyl-5-phenylimidazolidin-2,4-dione Pegoanone (. +/-)-Ethotoin
Inchi:	InChI=1S/C11H12N2O2/c1-2-13-10(14)9(12-11(13)15)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H
InchiKey:	SZQIFWWUIBRPBZ-UHFFFAOYSA-N
Formula:	C11H12N2O2
SMILES:	CCN1C(=O)NC(c2ccccc2)C1=O
Mol. weight [g/mol]:	204.23
CAS:	86-35-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	1.299		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1790.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86351&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

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