Paramethadione

Other names:	2,4-Oxazolidinedione, 5-ethyl-3,5-dimethyl- Paradione Parametadione A 348 3,5-Dimethyl-5-ethyloxazolidine-2,4-dione 5-Ethyl-3,5-dimethyloxazolidine-2,4-dione Isoethadione 5-Ethyl-3,5-dimethyl-2,4-oxazolidinedione
Inchi:	InChI=1S/C7H11NO3/c1-4-7(2)5(9)8(3)6(10)11-7/h4H2,1-3H3
InchiKey:	VQASKUSHBVDKGU-UHFFFAOYSA-N
Formula:	C7H11NO3
SMILES:	CCC1(C)OC(=O)N(C)C1=O
Mol. weight [g/mol]:	157.17
CAS:	115-67-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	0.764		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
rinpol	1120.00		NIST Webbook
tf	334.45 ± 0.50	K	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=C115673&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
tf:	Normal melting (fusion) point