

2H-3,1-Benzoxazine-2,4(1H)-dione, 1-methyl-

Other names:	N-Methylisatoic anhydride N-Methyl-N-carboxyanthranilic anhydride N-Methyl ia 2H-3,1-Benzoxazine-2,4(1H)-dione,N-methyl 1-methyl-2H-3,1-benzoxazine-2,4(1H)-dione
Inchi:	InChI=1S/C9H7NO3/c1-10-7-5-3-2-4-6(7)8(11)13-9(10)12/h2-5H,1H3
InchiKey:	KJMRWDHVBVCNLTQ-UHFFFAOYSA-N
Formula:	C9H7NO3
SMILES:	Cn1c(=O)oc(=O)c2ccccc21
Mol. weight [g/mol]:	177.16
CAS:	10328-92-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.14		Crippen Method
logp	0.492		Crippen Method
mcvol	122.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10328924&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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