

Methazole

Other names:	1,2,4-Oxadiazolidine-3,5-dione, 2-(3,4-dichlorophenyl)-4-methyl- 2-(3,4-Dichlorophenyl)-4-Methyl-1,2,4-oxadiazolidine-3,5-dione 2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidinedione Bioxone Chlormethazole Metazol Metazole Mezopur Oxydiazol Paxilon Probe Probe 75 Tunic VCS 438
Inchi:	InChI=1S/C9H6Cl2N2O3/c1-12-8(14)13(16-9(12)15)5-2-3-6(10)7(11)4-5/h2-4H,1H3
InchiKey:	LRUUNMYPIBZBQH-UHFFFAOYSA-N
Formula:	C9H6Cl2N2O3
SMILES:	<chem>Cn1c(=O)on(-c2ccc(Cl)c(Cl)c2)c1=O</chem>
Mol. weight [g/mol]:	261.06
CAS:	20354-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Aqueous Solubility Prediction Method
log10ws	-2.82		Estimated Solubility Method
logp	1.436		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
tf	397.03 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20354261&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

hfust: Enthalpy of fusion at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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