

Diclomezine

Other names:	3(2H)-Pyridazinone, 6-(3,5-dichloro-4-methylphenyl)-
Inchi:	InChI=1S/C11H8Cl2N2O/c1-6-8(12)4-7(5-9(6)13)10-2-3-11(16)15-14-10/h2-5H,1H3,(H,1
InchiKey:	UWQMKVBQKFHLCU-UHFFFAOYSA-N
Formula:	C11H8Cl2N2O
SMILES:	<chem>Cc1c(Cl)cc(-c2ccc(=O)[nH]n2)cc1Cl</chem>
Mol. weight [g/mol]:	255.10
CAS:	62865-36-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	2.570		Crippen Method
mcvol	168.640	ml/mol	McGowan Method
rinsol	2468.70		NIST Webbook
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Sources

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=C62865365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/16-122-8/Diclomezine.pdf>

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