

Imidazolidin-2,4-dione, 3-(3,5-dichlorophenyl)

Inchi:	InChI=1S/C9H6Cl2N2O2/c10-5-1-6(11)3-7(2-5)13-8(14)4-12-9(13)15/h1-3H,4H2,(H,12,1
InchiKey:	OGCORJSEYZKHIN-UHFFFAOYSA-N
Formula:	C9H6Cl2N2O2
SMILES:	O=C1CNC(=O)N1c1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	245.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	2.050		Crippen Method
mcvol	150.630	ml/mol	McGowan Method
rinpola	2464.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537578&Units=SI

Legend

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

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