

Imidazo[1,2-c]pyrimidine-5(1h)-thione, 1-(2-chloroethyl)-2,3-dihydro-

Inchi:	InChI=1S/C8H10CIN3S/c9-2-4-11-5-6-12-7(11)1-3-10-8(12)13/h1,3H,2,4-6H2
InchiKey:	CIJSNLDSRCPRLO-UHFFFAOYSA-N
Formula:	C8H10CIN3S
SMILES:	S=c1nccc2n1CCN2CCCI
Mol. weight [g/mol]:	215.70
CAS:	7151-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	1.671		Crippen Method
mcvol	147.490	ml/mol	McGowan Method

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=C7151759&Units=SI

Legend

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

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