

N-(2-chloroethyl)-n'-(7-quinolinyl)urea

Inchi:	InChI=1S/C12H12ClN3O/c13-5-7-15-12(17)16-10-4-3-9-2-1-6-14-11(9)8-10/h1-4,6,8H,5,
InchiKey:	ODPALQKHBXMXLF-UHFFFAOYSA-N
Formula:	C12H12ClN3O
SMILES:	O=C(NCCCl)Nc1ccc2cccnc2c1
Mol. weight [g/mol]:	249.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	2.595		Crippen Method
mcvol	180.470	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007809&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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