

Uracil, 1-{p-[3-(2-chloroethyl)ureido]benzyl}-

Inchi: InChI=1S/C14H15ClN4O3/c15-6-7-16-13(21)17-11-3-1-10(2-4-11)9-19-8-5-12(20)18-14(21)
InchiKey: BJODATBVEVQHPA-UHFFFAOYSA-N
Formula: C14H15ClN4O3
SMILES: O=C(NCCCCl)Nc1ccc(Cn2ccc(=O)[nH]c2=O)cc1
Mol. weight [g/mol]: 322.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	0.463		Crippen Method
mcvol	226.070	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=B6008383&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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