

Butethal permethylated

Inchi: InChI=1S/C13H22N2O3/c1-5-7-8-9-13(6-2)10(16)14(3)12(18)15(4)11(13)17/h5-9H2,1-4H
InchiKey: HETNCUKMJKEPDY-UHFFFAOYSA-N
Formula: C13H22N2O3
SMILES: CCCCC1(CC)C(=O)N(C)C(=O)N(C)C1=O
Mol. weight [g/mol]: 254.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	2.013		Crippen Method
mcvol	207.840	ml/mol	McGowan Method
rinpole	1564.00		NIST Webbook
rinpole	1564.00		NIST Webbook

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=R387838&Units=SI>

Legend

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

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