

Butethal perethylated

Inchi: InChI=1S/C15H26N2O3/c1-5-9-10-11-15(6-2)12(18)16(7-3)14(20)17(8-4)13(15)19/h5-11
InchiKey: ZCRFDJDIMMTXSM-UHFFFAOYSA-N
Formula: C15H26N2O3
SMILES: CCCCCC1(CC)C(=O)N(CC)C(=O)N(CC)C1=O
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.794		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
rinpol	1644.00		NIST Webbook
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Sources

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=R387823&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/116-345-0/Butethal-perethylated.pdf>

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