

Butethal perbutylated

Inchi: InChI=1S/C19H34N2O3/c1-5-9-12-13-19(8-4)16(22)20(14-10-6-2)18(24)21(17(19)23)15-
InchiKey: FSHNSRQEOYUPEG-UHFFFAOYSA-N
Formula: C19H34N2O3
SMILES: CCCCCC1(CC)C(=O)N(CCCC)C(=O)N(CCCC)C1=O
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	4.354		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
rinpol	1963.00		NIST Webbook

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=R387818&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/40-717-1/Butethal-perbutylated.pdf>

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