

Ethyltolylbarbital permethylated

Inchi: InChI=1S/C15H18N2O3/c1-5-15(11-8-6-10(2)7-9-11)12(18)16(3)14(20)17(4)13(15)19/h6
InchiKey: LONBWVQFBNGKDQ-UHFFFAOYSA-N
Formula: C15H18N2O3
SMILES: CCC1(c2ccc(C)cc2)C(=O)N(C)C(=O)N(C)C1=O
Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	1.693		Crippen Method
mcvol	212.260	ml/mol	McGowan Method
rinpol	1977.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R387863&Units=SI>

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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