

Butallylonal perbutylated

Inchi: InChI=1S/C19H31BrN2O3/c1-6-9-11-21-16(23)19(13-15(5)20,14(4)8-3)17(24)22(18(21)2
InchiKey: PSTREWJPKXFEIX-UHFFFAOYSA-N
Formula: C19H31BrN2O3
SMILES: C=C(Br)CC1(C(C)CC)C(=O)N(CCCC)C(=O)N(CCCC)C1=O
Mol. weight [g/mol]: 415.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	4.709		Crippen Method
mcvol	305.580	ml/mol	McGowan Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R387789&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

Latest version available from:

<https://www.chemeo.com/cid/14-784-6/Butallylonal-perbutylated.pdf>

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