

Allobarbitol perbutylated

Inchi: InChI=1S/C18H28N2O3/c1-5-9-13-19-15(21)18(11-7-3,12-8-4)16(22)20(17(19)23)14-10-
InchiKey: KDKNPSYYGLUITQ-UHFFFAOYSA-N
Formula: C18H28N2O3
SMILES: C=CCC1(CC=C)C(=O)N(CCCC)C(=O)N(CCCC)C1=O
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.516		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1894.00		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=R387709&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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.cheméo.com/cid/122-441-6/Allobarbitol-perbutylated.pdf>

Generated by Cheméo on 2024-05-09 04:38:42.157973281 +0000 UTC m=+17518771.078550600.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.