

Narcobarbital

Inchi: InChI=1S/C11H15BrN2O3/c1-6(2)11(5-7(3)12)8(15)13-10(17)14(4)9(11)16/h6H,3,5H2,1-
InchiKey: WGMASVSHOSNKMF-UHFFFAOYSA-N
Formula: C11H15BrN2O3
SMILES: C=C(Br)CC1(C(C)C)C(=O)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 303.15
CAS: 125-55-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.636		Crippen Method
mcvol	192.860	ml/mol	McGowan Method
rmpol	1814.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C125553&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/50-148-2/Narcobarbital.pdf>

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