

6-Butyroxytropan-3-ol

Inchi:	InChI=1S/C12H21NO3/c1-3-4-12(15)16-11-6-8-5-9(14)7-10(11)13(8)2/h8-11,14H,3-7H2,
InchiKey:	NXGHCTSWBFSTEJ-QPBDYMMBSA-N
Formula:	C12H21NO3
SMILES:	CCCC(=O)OC1CC2CC(O)CC1N2C
Mol. weight [g/mol]:	227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	0.926		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
rinsol	1634.00		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=R509934&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
rinsol:	Non-polar retention indices

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