

Temazepam o-propionyl deriv.

Other names:	Temazepam propanoate
Inchi:	InChI=1S/C19H17CIN2O3/c1-3-16(23)25-18-19(24)22(2)15-10-9-13(20)11-14(15)17(21)-
InchiKey:	XLLIZHAJTGQVQR-UHFFFAOYSA-N
Formula:	C19H17CIN2O3
SMILES:	CCC(=O)OC1N=C(c2ccccc2)c2cc(Cl)ccc2N(C)C1=O
Mol. weight [g/mol]:	356.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.433		Crippen Method
mcvol	257.100	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U281188&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/122-450-6/Tamazepam-o-propionyl-deriv.pdf>

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