Temazepam O-propionyl deriv.

Other names: Temazepam propanoate
Inchi: InChI=1S/C19H17ClN2O3/c1-3-16(23)25-18-19(24)22(2)15-10-9-13(20)11-14(15)17(21-1
InchiKey: XLLIZHAJTGQVQR-UHFFFAOYSA-N
Formula: C19H17ClN2O3
SMILES: CCC(=O)OC1N=C(c2ccccc2)c2cc(Cl)ccc2N(C)C1=O
Mol. weight [g/mol]: 356.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Cheméo Relay (1.0)
logp	3.433		Crippen Method
mcvol	257.100	ml/mol	McGowan Method
tf	397.62	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U281188&Units=SI
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
tf: Normal melting (fusion) point

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