

Quazepam

Other names:

2H-1,4-Benzodiazepine-2-thione,
7-chloro-5-(2-fluorophenyl)-1,3-dihydro-1-(2,2,2-trifluoroethyl)-
Sch 16134

7-Chloro-5-(o-fluorophenyl)-1,3-dihydro-1-(2,2,2-trifluoroethyl)-2H-1,4-benzodiazepine-2-

Dormalin

Doral

Oniria

Prosedar

Quazium

Selepam

Inchi: InChI=1S/C17H11ClF4N2S/c18-10-5-6-14-12(7-10)16(11-3-1-2-4-13(11)19)23-8-15(25)2**InchiKey:** IKMPWMZBZSAONZ-UHFFFAOYSA-N**Formula:** C17H11ClF4N2S**SMILES:** Fc1cccc1C1=NCC(=S)N(CC(F)(F)F)c2ccc(Cl)cc21**Mol. weight [g/mol]:** 386.79**CAS:** 36735-22-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	5.026		Crippen Method
mcvol	239.040	ml/mol	McGowan Method
rinsol	2485.00		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=C36735225&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
rinpol:	Non-polar retention indices

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