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-t
	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:	Fc1ccccc1C1=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
rinpol	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/ci990307l

Legend

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