

Halazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-1-(2,2,2-trifluoroethyl)- 2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-phenyl-1-(2,2,2-trifluoroethyl)- 7-Chloro-1,3-dihydro-5-phenyl-1-(2,2,2-trifluoroethyl)-2H-1,4-benzodiazepin-2-one ScH 12041 Schering 12041 Paxipam 7-Chloro-5-phenyl-1-(2,2,2-trifluoroethyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one Halezepam
Inchi:	InChI=1S/C17H12ClF3N2O/c18-12-6-7-14-13(8-12)16(11-4-2-1-3-5-11)22-9-15(24)23(14)
InchiKey:	WYCLKVQLVUQKNZ-UHFFFAOYSA-N
Formula:	C17H12ClF3N2O
SMILES:	O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1CC(F)(F)F
Mol. weight [g/mol]:	352.74
CAS:	23092-17-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	226.790	ml/mol	McGowan Method
rinpol	2292.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2337.10		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2337.10		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2335.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23092173&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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