etizolam

Inchi:	InChI=1S/C17H15ClN4S/c1-3-11-8-13-16(12-6-4-5-7-14(12)18)19-9-15-21-20-10(2)22(15
InchiKey:	VMZUTJCNQWMAGF-UHFFFAOYSA-N
Formula:	C17H15ClN4S
SMILES:	CCc1cc2c(s1)-n1c(C)nnc1CN=C2c1ccccc1Cl
Mol. weight [g/mol]:	342.85
CAS:	40054-69-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	4.204		Crippen Method
mcvol	241.060	ml/mol	McGowan Method
rinpol	3090.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40054691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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