Quazepam M (oxo-)

Other names: 2-oxoquazepam
Inchi: InChI=1S/C17H11ClF4N2O/c18-10-5-6-14-12(7-10)16(11-3-1-2-4-13(11)19)23-8-15(25)2
InchiKey: YFSXBSRGIRSXAD-UHFFFAOYSA-N
Formula: C17H11ClF4N2O
SMILES: O=C1CN=C(c2ccccc2F)c2cc(Cl)ccc2N1CC(F)(F)F
Mol. weight [g/mol]: 370.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.225		Crippen Method
mcvol	228.560	ml/mol	McGowan Method
rinpol	2255.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2255.00		NIST Webbook
rinpol	2270.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R313456&Units=SI

Legend

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