mexazolam

Inchi: InChI=1S/C18H16Cl2N2O2/c1-11-10-24-18(13-4-2-3-5-15(13)20)14-8-12(19)6-7-16(14)2
InchiKey: ANUCDXCTICZJRH-UHFFFAOYSA-N
Formula: C18H16Cl2N2O2
SMILES: CC1COC2(c3ccccc3Cl)c3cc(Cl)ccc3NC(=O)CN12
Mol. weight [g/mol]: 363.24
CAS: 31868-18-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	3.867		Crippen Method
mcvol	247.120	ml/mol	McGowan Method
rinpol	2670.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31868185&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.