

metaclozepam

Inchi: InChI=1S/C18H18BrClN2O/c1-22-13(11-23-2)10-21-18(14-5-3-4-6-16(14)20)15-9-12(19)
InchiKey: WABYCCJHARSRBH-UHFFFAOYSA-N
Formula: C18H18BrClN2O
SMILES: COCC1CN=C(c2ccccc2Cl)c2cc(Br)ccc2N1C
Mol. weight [g/mol]: 393.70
CAS: 65517-27-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	4.405		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
rinpol	2640.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2640.00		NIST Webbook
rinpol	2690.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65517273&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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