Fosazepam

Inchi: InChI=1S/C18H18ClN2O2P/c1-24(2,23)12-21-16-9-8-14(19)10-15(16)18(20-11-17(21)22
InchiKey: JMYCGCXYZZHWMO-UHFFFAOYSA-N
Formula: C18H18ClN2O2P
SMILES: CP(C)(=O)CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21
Mol. weight [g/mol]: 360.77
CAS: 35322-07-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	4.104		Crippen Method
mcvol	261.900	ml/mol	McGowan Method
rinpol	2605.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2610.00		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=C35322077&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

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