chlorbenzoylethamine

Other names: chlorbenzoyethamine
Inchi: InChI=1S/C28H32ClNO/c1-22-9-5-6-12-25(22)21-30-18-15-23(16-19-30)17-20-31-28(24-
InchiKey: KKGCLVWWIKWCBK-UHFFFAOYSA-N
Formula: C28H32ClNO
SMILES: Cc1ccccc1CN1CCC(CCOC(c2ccccc2)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 434.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.96		Crippen Method
logp	7.057		Crippen Method
mcvol	351.330	ml/mol	McGowan Method
rinpol	3255.00		NIST Webbook
rinpol	3170.00		NIST Webbook

Sources

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=R210956&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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