Cineroctine

Inchi: InChI=1S/C22H34N2O4/c1-2-3-5-17(25)11-22(27)28-18-8-9-23-13-15-10-16(20(23)12-18
InchiKey: SUVSPYYWRFXZNA-JREHQPMPSA-N
Formula: C22H34N2O4
SMILES: CCC=CC(O)CC(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 390.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	2.111		Crippen Method
mcvol	307.940	ml/mol	McGowan Method
rinpol	3170.00		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=R261291&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