Cacotheline

Inchi: InChI=1S/C20H21N3O7/c24-11-4-10-16(17(18(11)27)23(28)29)21-19-15-9-3-13-20(10,1
InchiKey: DLCUVFAXVOWNOS-UHFFFAOYSA-N
Formula: C20H21N3O7
SMILES: O=C(O)CC1OCC2CN3CCC45C6=CC(=O)C(=O)C([N+](=O)[O-])=C6NC4C1C2CC35
Mol. weight [g/mol]: 415.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	-0.275		Crippen Method
mcvol	272.730	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006085&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