Gynuramine

Inchi: InChI=1S/C18H25NO6/c1-3-11-8-13(9-20)18(2,23)17(22)24-10-12-4-6-19-7-5-14(15(12)1
InchiKey: XVKRSUITGOSAJK-OPJDVPNISA-N
Formula: C18H25NO6
SMILES: CC=C1CC(CO)C(C)(O)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.165		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
rinpol	2513.00		NIST Webbook
rinpol	2516.00		NIST Webbook
rinpol	2516.00		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=R178199&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