

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))
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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/44-056-1/Gynuramine.pdf>

Generated by Cheméo on 2024-04-19 22:35:54.067788662 +0000 UTC m=+15855402.988365983.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.