2-Pyridinecarbamic acid, 6-amino-4-[[2-hydroxy-3-(methylphenylamino)pro ethyl ester

InChI: InChI=1S/C18H24N6O5/c1-3-29-18(26)22-15-9-14(16(24(27)28)17(19)21-15)20-10-13(2

InChIKey: FBNXSOAJCFNWFD-UHFFFAOYSA-N

Formula: C18H24N6O5

SMILES: CCOC(=O)Nc1cc(NCC(O)CN(C)c2ccccc2)c([N+](=O)[O-])c(N)n1

Mol. weight [g/mol]: 404.42

CAS: 82585-86-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.050		Crippen Method
mcvol	297.590	ml/mol	McGowan Method

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=C82585862&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

Latest version available from:
https://www.chemeo.com/cid/73-865-1/2-Pyridinecarbamic-acid-6-amino-4-2-hydroxy-3-methylphenylamino-propyl-ar
Generated by Cheméo on 2024-04-26 07:17:11.121192273 +0000 UTC m=+16405080.041769584.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.