Nornicotine, N-octanoyl

Inchi: InChI=1S/C17H26N2O/c1-2-3-4-5-6-11-17(20)19-13-8-10-16(19)15-9-7-12-18-14-15/h7,9
InchiKey: KEQBTQJDZSZAMQ-UHFFFAOYSA-N
Formula: C17H26N2O
SMILES: CCCCCCCC(=O)N1CCCC1c1cccnc1
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	4.106		Crippen Method
mcvol	237.300	ml/mol	McGowan Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		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=R44857&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

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