

Trachelanthamidine

Inchi: InChI=1S/C8H15NO/c10-6-7-3-5-9-4-1-2-8(7)9/h7-8,10H,1-6H2/t7-,8?/m1/s1
InchiKey: LOFDEIYZIAVXHE-GVHYBUMESA-N
Formula: C8H15NO
SMILES: OCC1CCN2CCCC12
Mol. weight [g/mol]: 141.21
CAS: 526-64-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.66		Crippen Method
logp	0.463		Crippen Method
mcvol	117.710	ml/mol	McGowan Method
rinpola	1252.00		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=C526647&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/52-398-3/Trachelanthamidine.pdf>

Generated by Cheméo on 2024-04-25 19:30:38.344150817 +0000 UTC m=+16362687.264728132.

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