

Isonipecotic acid, N-methoxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-31-25(28)24-19
InchiKey: OYTPUODSGMTFTH-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	7.269		Crippen Method
mcvol	391.200	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322033&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/95-069-1/Isonipecotic-acid-N-methoxycarbonyl-octadecyl-ester.pdf>

Generated by Cheméo on 2025-12-05 14:36:24.474750177 +0000 UTC m=+4693582.004790834.

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