

Isonipecotic acid, N-ethoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-31-25(28)24-19-2
InchiKey: RJHBKGNJOIHIFM-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC)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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U322015&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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