

Pipecolic acid, N-propoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-23-30-25(28)24-20-17-1
InchiKey: TUPZWDJXVWLSKX-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.99		Crippen Method
logp	7.412		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
rmpol	3101.00		NIST Webbook
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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=U393007&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
rmpol: Non-polar retention indices

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