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: CCCCCCCCCCCCCCCCOC(=O)C1CCCCN1C(=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
rinpol	3101.00		NIST Webbook
rinpol	3101.00		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=U393007&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

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