Pipecolylpipecolic acid, N-propoxycarbonyl-, decyl ester

Inchi: InChI=1S/C26H46N2O5/c1-3-5-6-7-8-9-10-15-21-32-25(30)23-17-12-13-18-27(23)24(29)
InchiKey: KNKOHPXMJLRYLG-UHFFFAOYSA-N
Formula: C26H46N2O5
SMILES: CCCCCCCCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCC
Mol. weight [g/mol]: 466.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.34		Crippen Method
logp	5.452		Crippen Method
mcvol	391.890	ml/mol	McGowan Method
rinpol	3245.00		NIST Webbook
rinpol	3245.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393016&Units=SI
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

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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