

Pipecolylpipecolic acid, N-propoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C20H34N2O5/c1-3-5-15-26-19(24)17-11-7-8-12-21(17)18(23)16-10-6-9-13-22
InchiKey:	GIPMBLNCFJHYCA-UHFFFAOYSA-N
Formula:	C20H34N2O5
SMILES:	CCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCC
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	3.112		Crippen Method
mcvol	307.350	ml/mol	McGowan Method
rinpola	2650.00		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=U393010&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
rinpola:	Non-polar retention indices

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