

Pipecolic acid, N-propargyloxycarbonyl-, nonyl ester

Inchi: InChI=1S/C19H31NO4/c1-3-5-6-7-8-9-12-16-23-18(21)17-13-10-11-14-20(17)19(22)24-1
InchiKey: HYHJRWJZYLNMFV-UHFFFAOYSA-N
Formula: C19H31NO4
SMILES: C#CCOC(=O)N1CCCCC1C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	3.905		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
rinpole	2396.00		NIST Webbook
rinpole	2396.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393096&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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