Isonipecotic acid, N-isobutoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C18H33NO4/c1-4-5-6-7-8-13-22-17(20)16-9-11-19(12-10-16)18(21)23-14-15(2
InchiKey: CXRKEECLZHHRTD-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: CCCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	4.005		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2327.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322066&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