

Isonipecotic acid, N-isobutoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C17H31NO4/c1-13(2)6-5-11-21-16(19)15-7-9-18(10-8-15)17(20)22-12-14(3)4/
InchiKey: SEADBZKFPDPYKC-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	3.470		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinsol	2170.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322064&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinsol: Non-polar retention indices

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