

Isonipecotic acid, n-butoxycarbonyl-, octyl ester

Inchi: InChI=1S/C19H35NO4/c1-3-5-7-8-9-10-16-23-18(21)17-11-13-20(14-12-17)19(22)24-15
InchiKey: OLGVWUQHWXCQSV-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CCCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	4.539		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
rinpole	2473.00		NIST Webbook
rinpole	2473.00		NIST Webbook

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=U322053&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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