Isonipecotic acid, n-isobutoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C17H31NO4/c1-4-5-6-7-12-21-16(19)15-8-10-18(11-9-15)17(20)22-13-14(2)3/h
InchiKey: YHDGKSYQXUXECA-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]: 313.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Cheméo Relay (1.0)
logp	3.614		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2213.00		NIST Webbook
tb	627.22	K	Cheméo Relay (1.0)
tf	285.25	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322065&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point