Isonipecotic acid, n-isobutoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C23H43NO4/c1-4-5-6-7-8-9-10-11-12-13-18-27-22(25)21-14-16-24(17-15-21)2
InchiKey: CCNGTPRDBILBQN-UHFFFAOYSA-N
Formula: C23H43NO4
SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]: 397.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Cheméo Relay (1.0)
logp	5.955		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
rinpol	2859.00		NIST Webbook
rinpol	2859.00		NIST Webbook
tb	668.68	K	Cheméo Relay (1.0)
tf	302.40	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322071&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):
Cheméo Relay (1.0, beta):

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