Isonipecotic acid, N-ethoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C21H39NO4/c1-3-5-6-7-8-9-10-11-12-13-18-26-20(23)19-14-16-22(17-15-19)2

InchiKey: WVTALFUEVISTPB-UHFFFAOYSA-N

Formula: C21H39NO4

SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC)CC1

Mol. weight [g/mol]: 369.55

Physical Properties

Property code	Value	Unit	Source
hvap	112.14	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.92		Cheméo Relay (1.0)
logp	5.319		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rinpol	2682.00		NIST Webbook
tb	652.63	K	Cheméo Relay (1.0)
tf	296.37	K	Cheméo Relay (1.0)

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322011&Units=SI

Legend

hvap: Enthalpy of vaporization at standard conditions

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

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