Isonipecotic acid, N-ethoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-5-6-7-8-9-10-15-23-17(20)16-11-13-19(14-12-16)18(21)22-4
InchiKey: INMQONVHJBGFCK-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)OCC)CC1
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
hvap	100.22	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.92		Cheméo Relay (1.0)
logp	4.149		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	632.92	K	Cheméo Relay (1.0)
tf	285.88	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=U322008&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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