Isonipecotic acid, N-ethoxycarbonyl-, octyl ester

Inchi: InChI=1S/C17H31NO4/c1-3-5-6-7-8-9-14-22-16(19)15-10-12-18(13-11-15)17(20)21-4-2/h

InchiKey: QKZDHJOFYSFFTN-UHFFFAOYSA-N

Formula: C17H31NO4

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

Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
hvap	96.14	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.55		Cheméo Relay (1.0)
logp	3.759		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	625.81	K	Cheméo Relay (1.0)
tf	282.54	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322007&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

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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