

Isonipecotic acid, n-methoxycarbonyl-, hexadecyl ester

Inchi:	InChI=1S/C24H45NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-29-23(26)22-17-19-25
InchiKey:	SYWOSVPKZUHJRJ-UHFFFAOYSA-N
Formula:	C24H45NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]:	411.63

Physical Properties

Property code	Value	Unit	Source
hvap	124.57	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.92		Cheméo Relay (1.0)
logp	6.489		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
tb	668.55	K	Cheméo Relay (1.0)
tf	329.09		Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322031&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

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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