

Isonipecotic acid, N-(cyclohexylcarbonyl)-, ethyl ester

Inchi: InChI=1S/C15H25NO3/c1-2-19-15(18)13-8-10-16(11-9-13)14(17)12-6-4-3-5-7-12/h12-13
InchiKey: OJWMQRNBYOVBON-UHFFFAOYSA-N
Formula: C15H25NO3
SMILES: CCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 267.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	2.368		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
rinpola	2210.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361024&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/66-131-3/Isonipecotic-acid-N-cyclohexylcarbonyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-20 03:42:09.042973994 +0000 UTC m=+15873777.963551306.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.