

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

Inchi: InChI=1S/C20H35NO3/c1-2-3-4-5-9-16-24-20(23)18-12-14-21(15-13-18)19(22)17-10-7-6
InchiKey: QGKXCWWQJQXZKL-UHFFFAOYSA-N
Formula: C20H35NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 337.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	4.319		Crippen Method
mcvol	289.930	ml/mol	McGowan Method
rinpole	2740.00		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=U361030&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
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/47-295-3/Isonipecotic-acid-N-cyclohexylcarbonyl-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-26 19:24:45.337208088 +0000 UTC m=+16448734.257785406.

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