

Isonipecotic acid, N-(2-methoxybenzoyl)-, heptyl ester

Inchi: InChI=1S/C21H31NO4/c1-3-4-5-6-9-16-26-21(24)17-12-14-22(15-13-17)20(23)18-10-7-8
InchiKey: JOPBNFMBFFDAPF-UHFFFAOYSA-N
Formula: C21H31NO4
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1
Mol. weight [g/mol]: 361.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Crippen Method
logp	4.061		Crippen Method
mcvol	296.990	ml/mol	McGowan Method
rinpola	2911.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361191&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/64-925-4/Isonipecotic-acid-N-2-methoxybenzoyl-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-27 07:05:31.82350663 +0000 UTC m=+16490780.744083952.

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