

L-Proline, N-(furoyl-2)-, isohehexyl ester

Inchi: InChI=1S/C16H23NO4/c1-12(2)6-4-11-21-16(19)13-7-3-9-17(13)15(18)14-8-5-10-20-14/
InchiKey: YZKAUZAHHVYMMM-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1ccco1
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.74		Crippen Method
logp	2.864		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U346109&Units=SI>

Legend

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

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