

(2E,4E,10E)-1-(Piperidin-1-yl)hexadeca-2,4,10-trien-1-one

Inchi: InChI=1S/C21H35NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-21(23)22-19-16-14-17-20-21
InchiKey: MKTHMAHGEGGOMR-PJOYGNNGYSA-N
Formula: C₂₁H₃₅NO
SMILES: CCCCCC=CCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 317.51
CAS: 943546-16-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	5.808		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
rinpol	2792.30		NIST Webbook
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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=C943546165&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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