(2E,4E,12E)-1-(Piperidin-1-yl)octadeca-2,4,12-trien

Inchi: InChI=1S/C23H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23(25)24-21-18-16-19

InchiKey: HFWMTBWJCPVZTO-NMPGFTJCSA-N

Formula: C23H39NO

SMILES: CCCCCC=CCCCCCCC=CC=CC(=O)N1CCCCC1

Mol. weight [g/mol]: 345.56

CAS: 943546-19-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.25		Crippen Method
logp	6.588		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
rinpol	3014.80		NIST Webbook
rinpol	3014.80		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=C943546198&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

rinpol: Non-polar retention indices