

(2E,4E,14E)-1-(Piperidin-1-yl)icosa-2,4,14-trien-1-one

Inchi: InChI=1S/C25H43NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-25(27)26-23-24
InchiKey: XZJZLXUTPLOJRS-BESTWRNISA-N
Formula: C25H43NO
SMILES: CCCCCC=CCCCCCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 373.62
CAS: 943546-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.09		Crippen Method
logp	7.369		Crippen Method
mcvol	350.900	ml/mol	McGowan Method
rinpol	3213.60		NIST Webbook
rinpol	3213.60		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=C943546234&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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