

(2E,4E)-1-(Piperidin-1-yl)octadeca-2,4-dien-1-one

Inchi: InChI=1S/C23H41NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23(25)24-21-18-16-1
InchiKey: FCENBYBCTXRIOT-QDHVZSLHSA-N
Formula: C23H41NO
SMILES: CCCCCCCCCCCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 347.58
CAS: 151391-73-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.40 | | Crippen Method |
| logp | 6.812 | | Crippen Method |
| mcvol | 327.020 | ml/mol | McGowan Method |
| rinpol | 3033.00 | | NIST Webbook |
| rinpol | 3033.00 | | 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=C151391730&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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