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

Inchi: InChI=1S/C19H33NO/c1-2-3-4-5-6-7-8-9-10-11-13-16-19(21)20-17-14-12-15-18-20/h10-1
InchiKey: ARLNCELWGQDJPO-QDTXCPDVSA-N
Formula: C19H33NO
SMILES: CCCCCCCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 291.47
CAS: 52657-12-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	5.252		Crippen Method
mcvol	270.660	ml/mol	McGowan Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52657122&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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