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

Inchi: InChI=1S/C15H25NO/c1-2-3-4-5-6-7-9-12-15(17)16-13-10-8-11-14-16/h6-7,9,12H,2-5,8,1
InchiKey: ZPSGREUUQGTKDE-ZICOIJLXSA-N
Formula: C15H25NO
SMILES: CCCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 235.37
CAS: 42997-42-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	3.692		Crippen Method
mcvol	214.300	ml/mol	McGowan Method
rinpol	2149.60		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2140.00		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=C42997422&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

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