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

Inchi: InChI=1S/C17H29NO/c1-2-3-4-5-6-7-8-9-11-14-17(19)18-15-12-10-13-16-18/h8-9,11,14H
InchiKey: XNNQAABGMFGBSJ-HUKVCQRGSA-N
Formula: C17H29NO
SMILES: CCCCCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 263.42
CAS: 147030-06-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	4.472		Crippen Method
mcvol	242.480	ml/mol	McGowan Method
rinpol	2347.00		NIST Webbook
rinpol	2372.10		NIST Webbook
rinpol	2372.10		NIST Webbook
rinpol	2347.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C147030066&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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