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

Inchi: InChI=1S/C16H27NO/c1-2-3-4-5-6-7-8-9-10-13-16(18)17-14-11-12-15-17/h8-10,13H,2-7
InchiKey: UAIYHWLHQSKQLW-PEGOPYGQSA-N
Formula: C16H27NO
SMILES: CCCCCCCC=CC=CC(=O)N1CCCC1
Mol. weight [g/mol]: 249.39
CAS: 117137-69-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	4.082		Crippen Method
mcvol	228.390	ml/mol	McGowan Method
rinpol	2346.50		NIST Webbook
rinpol	2323.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C117137696&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