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

Inchi: InChI=1S/C21H37NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-21(23)22-19-16-14-17-20-2
InchiKey: UKCNPUUVSNIDBR-QOBMTOCASA-N
Formula: C21H37NO
SMILES: CCCCCCCCCCCC=CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 319.52
CAS: 486447-33-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.56		Crippen Method
logp	6.032		Crippen Method
mcvol	298.840	ml/mol	McGowan Method
rinpol	2802.80		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C486447330&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.