(E)-1-(Piperidin-1-yl)dodec-2-en-1-one

Inchi: InChI=1S/C17H31NO/c1-2-3-4-5-6-7-8-9-11-14-17(19)18-15-12-10-13-16-18/h11,14H,2-
InchiKey: VTWDGOQFLZYOQR-SDNWHVSQSA-N
Formula: C17H31NO
SMILES: CCCCCCCCCC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 265.43
CAS: 147030-03-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	4.696		Crippen Method
mcvol	246.780	ml/mol	McGowan Method
rinpol	2266.30		NIST Webbook
rinpol	2247.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C147030033&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