

(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: CCCCCCCCC=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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/90-212-6/E-1-Piperidin-1-yl-dodec-2-en-1-one.pdf>

Generated by Cheméo on 2024-04-26 08:42:06.21600069 +0000 UTC m=+16410175.136578003.

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