

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

Inchi: InChI=1S/C15H27NO/c1-2-3-4-5-6-7-9-12-15(17)16-13-10-8-11-14-16/h9,12H,2-8,10-11,15H
InchiKey: QBDDXKUFMFRNPR-FMIVXFBMSA-N
Formula: C15H27NO
SMILES: CCCCCC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 237.38
CAS: 147030-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.916		Crippen Method
mcvol	218.600	ml/mol	McGowan Method
rinpole	2051.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C147030022&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
rinpole: Non-polar retention indices

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