

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

Inchi: InChI=1S/C25H47NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-25(27)26-23-24
InchiKey: LWZQBNFYVPFFND-ZBJSNUHESA-N
Formula: C25H47NO
SMILES: CCCCCCCCCCCCCCCCCC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 377.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.38		Crippen Method
logp	7.817		Crippen Method
mcvol	359.500	ml/mol	McGowan Method
rinqol	3121.60		NIST Webbook

Sources

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=U413138&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinqol: Non-polar retention indices

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<https://www.chemeo.com/cid/95-432-7/E-1-Piperidin-1-yl-icos-2-en-1-one.pdf>

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