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

Inchi: InChI=1S/C23H43NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23(25)24-21-18-16-19
InchiKey: PPSREOHNKFETQU-LVZFUZTISA-N
Formula: C23H43NO
SMILES: CCCCCCCCCCCCCCCC=CC(=O)N1CCCCC1
Mol. weight [g/mol]: 349.59
CAS: 74267-81-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.54		Crippen Method
logp	7.036		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
rinpol	2893.70		NIST Webbook
rinpol	2893.70		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=C74267815&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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