

Cyclohexanone, 2-(ethylamino)-2-(2-thienyl)-

Other names:	Tiletamine
Inchi:	InChI=1S/C12H17NOS/c1-2-13-12(11-7-5-9-15-11)8-4-3-6-10(12)14/h5,7,9,13H,2-4,6,8H
InchiKey:	QAXBVGVYDCAVLV-UHFFFAOYSA-N
Formula:	C12H17NOS
SMILES:	CCNC1(c2cccs2)CCCCC1=O
Mol. weight [g/mol]:	223.33
CAS:	14176-49-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.696		Crippen Method
mcvol	177.520	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14176499&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

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<https://www.chemeo.com/cid/94-043-0/Cyclohexanone-2-ethylamino-2-2-thienyl.pdf>

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