

Acetamide, N-(1-naphthyl)-2-(2-thienyl)-

Inchi:	InChI=1S/C16H13NOS/c18-16(11-13-7-4-10-19-13)17-15-9-3-6-12-5-1-2-8-14(12)15/h1-
InchiKey:	FKIHEFZFNZEICZ-UHFFFAOYSA-N
Formula:	C16H13NOS
SMILES:	O=C(Cc1cccs1)Nc1cccc2ccccc12
Mol. weight [g/mol]:	267.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	4.083		Crippen Method
mcvol	201.520	ml/mol	McGowan Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306909&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

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<https://www.chemeo.com/cid/63-882-3/Acetamide-N-1-naphthyl-2-2-thienyl.pdf>

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