

Thiophene-2-carboxamide, N-ethyl-N-hexyl-

Inchi:	InChI=1S/C13H21NOS/c1-3-5-6-7-10-14(4-2)13(15)12-9-8-11-16-12/h8-9,11H,3-7,10H2,
InchiKey:	YXIKHPMQMUYSZ-UHFFFAOYSA-N
Formula:	C13H21NOS
SMILES:	CCCCCN(CC)C(=O)c1cccs1
Mol. weight [g/mol]:	239.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	3.790		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
rinsol	2054.00		NIST Webbook
rinsol	2054.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U415308&Units=SI

Legend

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

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