

2-Thiophenecarboxamide, N-(2-ethylhexyl)-

Inchi:	InChI=1S/C13H21NOS/c1-3-5-7-11(4-2)10-14-13(15)12-8-6-9-16-12/h6,8-9,11H,3-5,7,10
InchiKey:	SCXLTPDPNIQTIU-UHFFFAOYSA-N
Formula:	C13H21NOS
SMILES:	CCCCC(CC)CNC(=O)c1cccs1
Mol. weight [g/mol]:	239.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.694		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
rinpola	1993.00		NIST Webbook
rinpola	1993.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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