

Thiophene-2-carboxamide, N-ethyl-N-isobutyl-

Inchi:	InChI=1S/C11H17NOS/c1-4-12(8-9(2)3)11(13)10-6-5-7-14-10/h5-7,9H,4,8H2,1-3H3
InchiKey:	CFKVDHODMTWDOK-UHFFFAOYSA-N
Formula:	C11H17NOS
SMILES:	CCN(CC(C)C)C(=O)c1cccs1
Mol. weight [g/mol]:	211.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	2.866		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rmpol	1856.00		NIST Webbook
rmpol	1856.00		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=U415304&Units=SI

Legend

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

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