

2-Thiophenecarboxamide, N-isobutyl-

Inchi:	InChI=1S/C9H13NOS/c1-7(2)6-10-9(11)8-4-3-5-12-8/h3-5,7H,6H2,1-2H3,(H,10,11)
InchiKey:	PQGUJYPJCCMYFG-UHFFFAOYSA-N
Formula:	C9H13NOS
SMILES:	CC(C)CNC(=O)c1cccs1
Mol. weight [g/mol]:	183.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	2.134		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinsol	1613.00		NIST Webbook
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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=U407022&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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