Thiophene-2-carboxamide, N,N-diethyl-

Inchi: InChI=1S/C9H13NOS/c1-3-10(4-2)9(11)8-6-5-7-12-8/h5-7H,3-4H2,1-2H3
InchiKey: WCCLKHNWHBFKDF-UHFFFAOYSA-N
Formula: C9H13NOS
SMILES: CCN(CC)C(=O)c1cccs1
Mol. weight [g/mol]: 183.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	2.230		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U415302&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.