

3-Propyl thiophene-2-carboxaldehyde

Inchi:	InChI=1S/C8H10OS/c1-2-3-7-4-5-10-8(7)6-9/h4-6H,2-3H2,1H3
InchiKey:	LVILUBAIANFMFQ-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CCCc1ccsc1C=O
Mol. weight [g/mol]:	154.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.513		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
ripol	1839.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R547649&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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<https://www.chemeo.com/cid/88-281-3/3-Propyl-thiophene-2-carboxaldehyde.pdf>

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