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/ci990307l
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