3-ethyl-2-formylthiophene

Other names:	3-ethyl-2-thiophenecarboxaldehyde
	2-Thiophenecarboxaldehyde, 3-ethyl
Inchi:	InChI=1S/C7H8OS/c1-2-6-3-4-9-7(6)5-8/h3-5H,2H2,1H3
InchiKey:	ANIABPZLKNMRLN-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CCc1ccsc1C=O
Mol. weight [g/mol]:	140.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	2.123		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1206.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1206.00		NIST Webbook
ripol	1845.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R640416&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices