2-Furanacetaldehyde, «alpha»-propyl-

Other names: 2-(2-Furyl)pentanal
Inchi: InChI=1S/C9H12O2/c1-2-4-8(7-10)9-5-3-6-11-9/h3,5-8H,2,4H2,1H3
InchiKey: VABVMGKHVDVOBI-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CCCC(C=O)c1ccco1
Mol. weight [g/mol]: 152.19
CAS: 31681-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.51		Crippen Method
logp	2.362		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		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=C31681262&Units=SI

Legend

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

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