

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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