2-Furanacetaldehyde, «alpha»-methyl-«alpha»-vinyl-

Other names: 2-(2-Furyl)-2-methyl-3-butenal
«alpha»-Methyl-«alpha»-vinyl-2-furanacetaldehyde
Inchi: InChI=1S/C9H10O2/c1-3-9(2,7-10)8-5-4-6-11-8/h3-7H,1H2,2H3
InchiKey: PLLOKKQQTSGSSC-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: C=CC(C)(C=O)c1ccco1
Mol. weight [g/mol]: 150.17
CAS: 31776-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	1.922		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
ripol	1837.00		NIST Webbook
ripol	1837.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31776280&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
ripol: Polar retention indices