

2-Furancarboxylic acid, propyl ester

Other names:	2-Furoic acid, propyl ester Propyl 2-furoate n-Propyl furoate Propyl furoate 2-Furoic acid, n-propyl ester
Inchi:	InChI=1S/C8H10O3/c1-2-5-11-8(9)7-4-3-6-10-7/h3-4,6H,2,5H2,1H3
InchiKey:	HSCVIIIISAAEVQT-UHFFFAOYSA-N
Formula:	C8H10O3
SMILES:	CCCOC(=O)c1ccco1
Mol. weight [g/mol]:	154.16
CAS:	615-10-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	1.846		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
ripol	1125.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615101&Units=SI
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

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

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