

2-Furancarboxylic acid, pentadecyl ester

Other names:	Pentadecyl 2-furancarboxylic acid
Inchi:	InChI=1S/C20H34O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-23-20(21)19-16-15-18-22-19
InchiKey:	UCZLSNQPQXBXSK-UHFFFAOYSA-N
Formula:	C20H34O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccco1
Mol. weight [g/mol]:	322.48
CAS:	220876-47-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.31		Crippen Method
logp	6.528		Crippen Method
mcvol	286.510	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220876471&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

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