

Lecithin

Other names:	Lecithins
Inchi:	InChI=1S/C44H86NO8P/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-36-43(46)50-4
InchiKey:	ATHVAWFVAEPLPPQ-LNVKXUELSA-N
Formula:	C44H86NO8P
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OC(COC(=O)CCCCCCCCCCCCCCCCC)COP(=O)([O
Mol. weight [g/mol]:	788.13
CAS:	8002-43-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.27		Crippen Method
logp	11.948		Crippen Method
mcvol	695.320	ml/mol	McGowan Method
rinpola	2147.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C8002435&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
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/71-055-2/Lecithin.pdf>

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