Trioctadecoxyborane (n)

Inchi:	InChI=1S/C54H111BO3/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-56-55(5
InchiKey:	GZKLCETYSGSMRA-UHFFFAOYSA-N
Formula:	C54H111BO3
SMILES:	CCCCCCCCCCCCCCCCCCOB(OCCCCCCCCCCCCCCCCCC)OCCCCCCCCCCCCCC
Mol. weight [g/mol]:	819.27
CAS:	5337-41-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-18.94		Crippen Method
logp	19.806		Crippen Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5337417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

Latest version available from:

https://www.chemeo.com/cid/79-943-8/Trioctadecoxyborane-n.pdf

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