

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

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/79-943-8/Trioctadecoxyborane-n.pdf>

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