

Silane, diphenylheptyloxy(1,1,1-trifluoro-3-bromoprop-2-yloxy)

Inchi: InChI=1S/C22H28BrF3O2Si/c1-2-3-4-5-12-17-27-29(19-13-8-6-9-14-19,20-15-10-7-11-10)/1
InchiKey: LQEJEGMYICHEJM-UHFFFAOYSA-N
Formula: C22H28BrF3O2Si
SMILES: CCCCCCO[Si](OC(CBr)C(F)(F)F)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 489.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.21		Crippen Method
logp	5.572		Crippen Method
rinpol	2340.00		NIST Webbook

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=U368085&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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