

Octylbis(trifluoromethyl)phosphine sulfide

Other names:	Octyl bis(trifluoromethyl)thiophosphine
Inchi:	InChI=1S/C10H17F6PS/c1-2-3-4-5-6-7-8-17(18,9(11,12)13)10(14,15)16/h2-8H2,1H3
InchiKey:	CBZUJGNVEMAUCM-UHFFFAOYSA-N
Formula:	C10H17F6PS
SMILES:	CCCCCCCCP(=S)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	314.27
CAS:	136338-51-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	5.866		Crippen Method
mcvol	199.190	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136338517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/79-709-8/Octylbis-trifluoromethyl-phosphine-sulfide.pdf>

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