

Hexabutylthiophosphoramide

Inchi:	InChI=1S/C24H54N3PS/c1-7-13-19-25(20-14-8-2)28(29,26(21-15-9-3)22-16-10-4)27(23-
InchiKey:	MAEYAXJKWCYNNG-UHFFFAOYSA-N
Formula:	C24H54N3PS
SMILES:	CCCCN(CCCC)P(=S)(N(CCCC)CCCC)N(CCCC)CCCC
Mol. weight [g/mol]:	447.74
CAS:	3949-47-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	7.918		Crippen Method
mcvol	415.770	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3949471&Units=SI

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/83-985-7/Hexabutylthiophosphoramide.pdf>

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