

Trimethylphosphine sulfide

Inchi:	InChI=1S/C3H9PS/c1-4(2,3)5/h1-3H3
InchiKey:	KTFAZNVGJUIWJM-UHFFFAOYSA-N
Formula:	C3H9PS
SMILES:	CP(C)(C)=S
Mol. weight [g/mol]:	108.14
CAS:	2404-55-9

Physical Properties

Property code	Value	Unit	Source
ie	8.48	eV	NIST Webbook
ie	8.48 ± 0.04	eV	NIST Webbook
log10ws	3.64		Crippen Method
logp	1.355		Crippen Method
mcvol	89.940	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	70.30	kJ/mol	380.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C2404559&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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