Triphenylphosphine sulfide

Other names:	Phosphine sulfide, triphenyl- (C6H5)3P=S Triphenylphosphorus sulfide (C6H5)3PS triphenylphosphine sulphide
Inchi:	InChI=1S/C18H15PS/c20-19(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1
InchiKey:	VYNGFCUGSYEOOZ-UHFFFAOYSA-N
Formula:	C18H15PS
SMILES:	S=P(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	294.35
CAS:	3878-45-3

Physical Properties

Property code	Value	Unit	Source
affp	906.20	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
hsub	142.80 ± 6.80	kJ/mol	NIST Webbook
log10ws	-13.11		Crippen Method
logp	3.442		Crippen Method
mcvol	230.010	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	136.80 ± 6.10	kJ/mol	403.50	NIST Webbook

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

Legend

affp:	Proton affinity
basg:	Gas basicity
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume