

Tricyanophosphine

Inchi:	InChI=1S/C3N3P/c4-1-7(2-5)3-6
InchiKey:	VXFKMOLPHLQGLH-UHFFFAOYSA-N
Formula:	C3N3P
SMILES:	N#CP(C#N)C#N
Mol. weight [g/mol]:	109.03
CAS:	1116-01-4

Physical Properties

Property code	Value	Unit	Source
hsub	75.30 ± 2.90	kJ/mol	NIST Webbook
log10ws	1.98		Crippen Method
logp	0.912		Crippen Method
mcvol	77.730	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	78.30	kJ/mol	308.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1116014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/52-042-7/Tricyanophosphine.pdf>

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