

Phosphine, tris(4-methylphenyl)-

Other names:

Phosphine, tri-p-tolyl-
Tri-p-tolylphosphine
Tris(p-tolyl)phosphine
Tris(4-methylphenyl)phosphine
Tris(4-tolyl)phosphine
Phosphorus, tri-p-tolyl
tri-(4-Methylphenyl)phosphine
tri(4-Tolyl)phosphine
Phosphine, tris(p-tolyl)-
Tri-para-tolylphosphine
Tris(p-methylphenyl)phosphine
NSC 97371

Inchi:

InChI=1S/C21H21P/c1-16-4-10-19(11-5-16)22(20-12-6-17(2)7-13-20)21-14-8-18(3)9-15-

InchiKey:

WXAZIUYTQHYBFW-UHFFFAOYSA-N

Formula:

C₂₁H₂₁P

SMILES:

Cc1ccc(P(c2ccc(C)cc2)c2ccc(C)cc2)cc1

Mol. weight [g/mol]:

304.37

CAS:

1038-95-5

Physical Properties

Property code	Value	Unit	Source
ie	7.60	eV	NIST Webbook
log10ws	-15.11		Crippen Method
logp	4.370		Crippen Method
mvol	255.930	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	126.00 ± 5.00	kJ/mol	383.00	NIST Webbook

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=C1038955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization 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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