Bis-(1,3-diphenylphosphino)propane

Other names: Bis(1,3-diphenylphosphino)propane
Phosphine, 1,3-propanediylbis[diphenyl-
Phosphine, trimethylenebis(diphenyl-
Trimethylenebis(diphenylphosphine)
1,3-Propanediylbis(diphenylphosphine)
propane-1,3-diylbis(diphenylphosphine)

Inchi: InChI=1S/C27H26P2/c1-5-14-24(15-6-1)28(25-16-7-2-8-17-25)22-13-23-29(26-18-9-3-10

InchiKey: LVEYOSJUKRVCCF-UHFFFAOYSA-N

Formula: C27H26P2

SMILES: c1ccc(P(CCCP(c2ccccc2)c2ccccc2)c2ccccc2)cc1

Mol. weight [g/mol]: 412.45

Physical Properties

Property code	Value	Unit	Source
ie	7.92	eV	Cheméo Relay (1.0)
logp	5.642		Crippen Method
mcvol	337.170	ml/mol	McGowan Method
tf	393.69	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6737424&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point