1,4-Bis(diphenylphosphino)butane

Other names: Phosphine, 1,4-butanediylbis[diphenyl-
Butane-1,4-diylbis(diphenylphosphine)
Inchi: InChI=1S/C28H28P2/c1-5-15-25(16-6-1)29(26-17-7-2-8-18-26)23-13-14-24-30(27-19-9-3
InchiKey: BCJVBDBJSMFBRW-UHFFFAOYSA-N
Formula: C28H28P2
SMILES: c1ccc(P(CCCCP(c2ccccc2)c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 426.47
CAS: 7688-25-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-17.21		Crippen Method
logp	6.032		Crippen Method
mcvol	351.260	ml/mol	McGowan Method
tf	405.90 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	354.00	J/mol×K	364.00	NIST Webbook
hfust	45.30	kJ/mol	405.90	NIST Webbook
hfust	45.30	kJ/mol	405.90	NIST Webbook
hsubt	171.60	kJ/mol	443.00	NIST Webbook
hsubt	171.60 ± 2.50	kJ/mol	440.00	NIST Webbook
hvapt	126.00 ± 2.00	kJ/mol	440.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7688257&Units=SI
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

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point