Phosphorodiamidothioic chloride, tetramethyl-

Other names:	Tetramethyldiamidothiophosphoryl chloride
	Tetramethylphosphorodiamidothioic chloride
	Bis(dimethylamino)phosphinothioic chloride
	N,N,N',N'-Tetramethylphosphorodiamidothioic chloride
	Bis(dimethylamino)chlorophosphine sulfide
Inchi:	InChI=1S/C4H12ClN2PS/c1-6(2)8(5,9)7(3)4/h1-4H3
InchiKey:	CDAZTLZRVPHQHS-UHFFFAOYSA-N
Formula:	C4H12ClN2PS
SMILES:	CN(C)P(=S)(Cl)N(C)C
Mol. weight [g/mol]:	186.64
CAS:	3732-81-8

Physical Properties

Property code	Value	Unit	Source
ie	8.23 ± 0.02	eV	NIST Webbook
ie	8.23 ± 0.00	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
log10ws	2.96		Crippen Method
logp	1.573		Crippen Method
mcvol	136.230	ml/mol	McGowan Method
tf	295.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.50 ± 0.50	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3732818&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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/33-102-1/Phosphorodiamidothioic-chloride-tetramethyl.pdf
Generated by Cheméo on 2024-04-26 19:03:23.463953153 +0000 UTC m=+16447452.384530469.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.