

Phosphorodichloridothioamide, n-methyl-

Inchi:	InChI=1S/CH4Cl2NPS/c1-4-5(2,3)6/h1H3,(H,4,6)
InchiKey:	HPEXXKFLWCBICT-UHFFFAOYSA-N
Formula:	CH4Cl2NPS
SMILES:	CNP(=S)(Cl)Cl
Mol. weight [g/mol]:	163.99
CAS:	20665-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	2.01		Crippen Method
logp	1.908		Crippen Method
mcvol	96.220	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20665230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/26-596-2/Phosphorodichloridothioamide-n-methyl.pdf>

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