

# Temefos

## Other names:

AC 52160  
Abat  
Abate  
Abate 4-E  
Abathion  
American cyanamid AC 52,160  
American cyanamid CL-52160  
American cyanamid E.I. 52,160  
Biothion  
Biothon  
Bithion  
CL 52160  
Difenphos  
Difos  
Diphos  
Diphos (Pesticide)  
EI 52160  
ENT 27,165  
Ecopro 1707  
Experimental Insecticide 52,160  
Experimental Insecticide 52160  
Nephis  
Nephis 1G  
Nimitex  
Nimitox  
O,O'-(Thiodi-4,1-phenylene)bis(O,O-dimethyl phosphorothioate)  
O,O'-(Thiodi-4,1-phenylene)phosphorothioic acid O,O,O',O'-tetramethyl ester  
O,O'-(Thiodi-p-phenylene) O,O,O',O'-tetramethyl bis(phosphorothioate)  
O,O,O',O'-Tetramethyl O,O'-(Thiodi-p-phenylene) phosphorothioate  
O,O,O',O'-tetramethyl O,O'-thiodi-p-phenylene bis(phosphorothioate)  
O,O-Dimethyl phosphorothioate O,O-diester with 4,4'-thiodiphenol  
Phenol, 4,4'-thiodi-, O,O-diester with O,O-dimethyl phosphorothioate  
Phosphorothioic acid, O,O'-(thiodi-4,1-phenylene) O,O,O',O'-tetramethyl ester  
Phosphorothioic acid, O,O'-(thiodi-p-phenylene) O,O,O',O'-tetramethyl ester  
Phosphorothioic acid, O,O-dimethyl ester, O,O-diester with 4,4'-thiodiphenol  
Phosphorothioic acid, Op,Op'-(thiodi-4,1-phenylene) Op,Op,Op',Op'-tetramethyl ester  
Procida  
Swebate  
Temephos  
Temophos

**Inchi:** Tetramethyl-O,O'-thiodi-p-phenylene phosphorothioate  
**InchiKey:** InChI=1S/C16H20O6P2S3/c1-17-23(25,18-2)21-13-5-9-15(10-6-13)27-16-11-7-14(8-12-13)/p1  
**Formula:** WWJZWCUNLNYYAU-UHFFFAOYSA-N  
**SMILES:** C16H20O6P2S3  
**SMILES:** COP(=S)(OC)Oc1ccc(Sc2ccc(OP(=S)(OC)OC)cc2)cc1  
**Mol. weight [g/mol]:** 466.47  
**CAS:** 3383-96-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Aqueous Solubility Prediction Method
log10ws	-6.24		Estimated Solubility Method
logp	5.630		Crippen Method
mcvol	313.970	ml/mol	McGowan Method
tf	304.42 ± 0.20	K	NIST Webbook
tf	305.00 ± 0.20	K	NIST Webbook
tf	303.40	K	Aqueous Solubility Prediction Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.03	kJ/mol	303.20	NIST Webbook

## Sources

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3383968&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

# Legend

<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tf:</b>	Normal melting (fusion) point

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