

Thiotepa

Other names:

Aziridine, 1,1',1''-phosphinothioylidynetris-
CBC 806495
Girostan
N,N',N''-Tri-1,2-ethanediylphosphorothioic triamide
N,N',N''-Tri-1,2-ethanediylthiophosphoramide
N,N',N''-Triethylenephosphorothioic triamide
N,N',N''-Triethylenethiophosphamide
N,N',N''-Triethylenethiophosphoramide
NCI-C01649
NSC 6396
Oncotepa
Oncothio-tepa
Oncotiotepa
Phosphine sulfide, tris(1-aziridiny)-
Phosphorothioic acid triethylenetriamide
Phosphorothioic triamide, N,N',N''-tri-1,2-ethanediyl-
Phosphorothioic triamide, N,N',N''-triethylene
SK 6882
STEPS
Tepa
Tespamin
Tespamine
Thio-tepa S
Thio-Tep
Thiofozil
Thiophosphamide
Thiophosphoramide, N,N',N''-triethylene-
Thiophosphoramide, N,N',N''-tri-1,2-ethanediyl-
Thiotef
Thiotriethylenephosphoramide
Tifosyl
Tio-tef
Tiofosamid
Tiofosyl
Tiofozil
Tri(ethyleneimino)thiophosphoramide
Triaziridinylphosphine sulfide
Triethylene thiophosphoramide
Triethylenethiophosphorotriamide
Tris(ethylenimino)thiophosphate

Tris(1-aziridinyl)phosphine sulfide
TSPA
1,1',1''-Phosphinothioylidynetrisaziridine
Phosphorothioic triamide, N,N',N''-triethylene-
Tris(1-aziridinyl)phosphine sulphide
Tris(aziridinyl)phosphine sulfide
Thioplex
N,N',N''-Triethylenethiophosphortriamide
Tri-1-aziridinylphosphine sulfide
AI 3-24916

Inchi: InChI=1S/C6H12N3PS/c11-10(7-1-2-7,8-3-4-8)9-5-6-9/h1-6H2
InchiKey: FOCVUCIESVLUNU-UHFFFAOYSA-N
Formula: C6H12N3PS
SMILES: S=P(N1CC1)(N1CC1)N1CC1
Mol. weight [g/mol]: 189.22
CAS: 52-24-4

Physical Properties

Property code	Value	Unit	Source
log10ws	4.02		Crippen Method
logp	0.158		Crippen Method
mcvol	129.570	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C52244&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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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