Triaziquone

Other names:

2,5-Cyclohexadiene-1,4-dione, 2,3,5-tris(1-aziridinyl)-
p-Benzoquinone, tris(1-aziridinyl)-
p-Benzoquinone, 2,3,5-tris(1-aziridinyl)-
A 163
Aziridine, 1,1',1''-(3,6-dioxo-1,4-cyclohexadiene-1,2,4-triyl)tris-
Bayer 3231
BAY 3231
NSC-29215
Oncoredox
Oncovedex
Prenimon
Riker 601
Trenimon
Treninon
Triazichon
Triaziquinone
Triaziquon
Triethyleneaminobenzoquinone
Triethyleneiminobenzoquinone
Triethyleniminobenzoquinone
Tris(aziridinyl)-p-benzoquinone
Tris(ethyleneimino)benzoquinone
Tris(1-aziridinyl)-p-benzoquinone
Trisaethyleniminobenzochinon
Trisethyleneiminoquinone
TEIB
1,1',1''-(3,6-Dioxo-1,4-cyclohexadiene-1,2,4-triyl)trisaziridine
10257 R.P.
2,3,5-Ethylenimine-1,4-benzoquinone
2,3,5-Tri(1-aziridinyl)-p-benzoquinone
2,3,5-Triethyleneimino-p-benzoquinone
2,3,5-Triethyleneimino-1,4-benzoquinone
2,3,5-Tris(aziridino)-1,4-benzoquinone
2,3,5-Tris(aziridinyl)-1,4-benzoquinone
2,3,5-Tris(ethyleneimino)benzoquinone
2,3,5-Tris(ethylenimino)-p-benzoquinone
2,3,5-Tris(ethylenimino)-1,4-benzoquinone
2,3,5-Tris(ethylenimino)benzoquinone
2,3,5-Tris(1-aziridino)-p-benzoquinone
2,3,5-Tris(1-aziridinyl)-2,5-cyclohexadiene-1,4-dione

	Triaziquonum
Inchi:	InChI=1S/C12H13N3O2/c16-9-7-8(13-1-2-13)12(17)11(15-5-6-15)10(9)14-3-4-14/h7H,1-
InchiKey:	PXSOHRWMIRDKMP-UHFFFAOYSA-N
Formula:	C12H13N3O2
SMILES:	O=C1C=C(N2CC2)C(=O)C(N2CC2)=C1N1CC1
Mol. weight [g/mol]:	231.25
CAS:	68-76-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.11		Crippen Method
logp	-0.819		Crippen Method
mcvol	160.980	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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