Razoxane

Other names:	.+/-.-(3,5,3',5'-Tetraoxo)-1,2-dipiperazinopropane
	(.+/-.)-1,2-Bis(3,5-dioxopiperazinyl)propane
	ICRF 159
	NSC 129943
	Propane, (.+/-.)-1,2-bis(3,5-dioxopiperazin-1-yl)-
	Razoxin
	2,6-Piperazinedione, 4,4'-(1-methyl-1,2-ethanediyl)bis-, (.+/-.)-
	2,6-Piperazinedione, 4,4'-propylenedi-
	2,6-Piperazinedione, 4,4'-propylenedi-, (.+/-.)-
	(.+/-.)-1,2-Bis(3,5-dioxopiperazine-1-yl)propane
	NCI-C01627
	(.+/-.)-4,4'-Propylenedi-2,6-piperazinedione
	(.+/-.)-Razoxane
	ICI-59118
	1,2-Bis(3,5-dioxo-1-piperazinyl)propane
	2,6-Piperazinedione, 4,4'-(1-methyl-1,2-ethanediyl)bis-
	4,4'-Propylenebis(2,6-piperazinedione)
	Tepirone
	Troxozone
	4,4'-propylenebis(piperazine-2,6-dione)
	(+) 4,4'-(1-Methyl-1,2-ethanediyl)bis-2,6-piperazinedione (dexrazoxane)
Inchi:	InChI=1S/C11H16N4O4/c1-7(15-5-10(18)13-11(19)6-15)2-14-3-8(16)12-9(17)4-14/h7H,2
InchiKey:	BMKDZUISNHGIBY-UHFFFAOYSA-N
Formula:	C11H16N4O4
SMILES:	CC(CN1CC(=O)NC(=O)C1)N1CC(=O)NC(=O)C1
Mol. weight [g/mol]:	268.27
CAS:	21416-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.05		Crippen Method
logp	-2.708		Crippen Method
mcvol	190.330	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	44.98	kJ/mol	507.40	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21416671&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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