Quinomethionate

Other names:	1,3-Dithiolo[4,5-b]quinoxalin-2-one, 6-methyl-
	Carbonic acid, dithio-, cyclic S,S-(6-methyl-2,3-quinoxalinediyl) ester
	Bayer 4964
	BAY 36205
	Chinomethionat
	Forstan
	Morestan
	Morestane
	MQD
	Oxythioquinox
	6-Methyl-1,3-Dithiolo[4,5-b]quinoxalin-2-one
	6-Methyl-2,3-quinoxalinedithiol cyclic carbonate
	6-Methyl-2,3-quinoxalinedithiol cyclic dithiocarbonate
	Chinomethionate
	ENT 25606
	SS 2074
	Quinomethionat
	6-Methyl-2,3-quinoxalinedithiol cyclic S,S-dithiocarbonate
	6-Methyl-2-oxo-1,3-dithio[4,5-b]quinoxaline
	Bayer 36205
	Carbonic acid, dithio-, cyclic S,S-ester with 6-methyl-2,3-quinoxalinedithiol
	Cetactaelate
	Daisonet XL 21
	Morestan 2
	NSC 379587
Inchi:	InChI=1S/C10H6N2OS2/c1-5-2-3-6-7(4-5)12-9-8(11-6)14-10(13)15-9/h2-4H,1H3
InchiKey:	FBQQHUGEACOBDN-UHFFFAOYSA-N
Formula:	C8H6N2OS2
SMILES:	Cc1ccc2nc3sc(=O)sc3nc2c1
Mol. weight [g/mol]:	210.28
CAS:	2439-01-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	2.575		Crippen Method

mcvol	151.910	ml/mol	McGowan Method
rinpol	2081.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tf	443.68 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.92	kJ/mol	443.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2439012&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point