Molinate

Other names:	1H-Azepine-1-carbothioic acid, hexahydro-, S-ethyl ester
	Ethyl 1-hexamethyleneiminecarbothiolate
	Felan
	Hydram
	Jalan
	Molmate
	Ordram
	R-4572
	S-Aethyl-N-hexahydro-1H-azepinthiolcarbamat
	S-Ethyl 1-hexamethyleneiminothiocarbamate
	S-Ethyl Hexahydroazepine-1-carbothioate
	S-Ethyl N,N-hexamethylenethiocarbamate
	S-Ethyl N,N-hexamethylenothiocarbamate
	S-Ethyl azepane-1-carbothioate
	S-Ethyl hexahydro-1H-azepine-1-carbothioate
	S-Ethyl-N-hexamethylenethiocarbamate
	Stauffer R-4,572
	Yalan
	Yulan
Inchi:	InChI=1S/C9H17NOS/c1-2-12-9(11)10-7-5-3-4-6-8-10/h2-8H2,1H3
InchiKey:	DEDOPGXGGQYYMW-UHFFFAOYSA-N
Formula:	C9H17NOS
SMILES:	CCSC(=O)N1CCCCCC1
Mol. weight [g/mol]:	187.30
CAS:	2212-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Aqueous Solubility Prediction Method
logp	2.736		Crippen Method
mcvol	154.710	ml/mol	McGowan Method
rinpol	1539.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1533.00		NIST Webbook

rinpol	1538.00	NIST Webbook
rinpol	1547.00	NIST Webbook
rinpol	1547.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2212671&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices