2H-thiopyran-4-imine, n-hydroxy-tetrahydro-1,1-dioxide

Inchi: InChI=1S/C5H9NO3S/c7-6-5-1-3-10(8,9)4-2-5/h7H,1-4H2
InchiKey: XLHSBMADTKQVET-UHFFFAOYSA-N
Formula: C5H9NO3S
SMILES: O=S1(=O)CCC(=NO)CC1
Mol. weight [g/mol]: 163.19
CAS: 99586-63-7

Physical Properties

Property code	Value	Unit	Source
hf	-633.03	kJ/mol	Joback Method
hvap	65.91	kJ/mol	Joback Method
log10ws	0.54		Crippen Method
logp	0.025		Crippen Method
mcvol	110.090	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
tb	536.19	K	Joback Method
tc	736.58	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99586637&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature