

Thiosulfuric acid (H₂S₂O₃), S-[2-[(tetrahydro-1,1-dioxido-3-thienyl)amino]ethyl] ester

Other names:
ester

Ethanethiosulfonic acid, 2-amino-N-(1,1-dioxotetrahydrothiophen-3-yl)-

Thiosulfuric acid, S-[2-[(tetrahydro-1,1-dioxido-3-thienyl)amino]ethyl] ester

Inchi: InChI=1S/C6H13NO5S3/c8-14(9)4-1-6(5-14)7-2-3-13-15(10,11)12/h6-7H,1-5H2,(H,10,11)

InchiKey: XJZPIFAXYFWKTO-ZCFIWIBFSA-N

Formula: C₆H₁₃NO₅S₃

SMILES: O=S1(=O)CCC(NCCSS(=O)(=O)O)C1

Mol. weight [g/mol]: 275.37

CAS: 37018-35-2

Physical Properties

Property code	Value	Unit	Source
gf	-908.46	kJ/mol	Joback Method
hf	-1066.89	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	95.40	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	-0.701		Crippen Method
mvol	172.920	ml/mol	McGowan Method
pc	6886.93	kPa	Joback Method
tb	637.70	K	Joback Method
tc	828.02	K	Joback Method
tf	442.33	K	Joback Method
vc	0.664	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.92	J/mol×K	637.70	Joback Method
cpg	453.04	J/mol×K	669.42	Joback Method
cpg	464.37	J/mol×K	701.14	Joback Method
cpg	474.91	J/mol×K	732.86	Joback Method
cpg	484.67	J/mol×K	764.58	Joback Method
cpg	493.64	J/mol×K	796.30	Joback Method
cpg	501.82	J/mol×K	828.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37018352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/19-619-4/Thiosulfuric-acid-H2S2O3-S-2-tetrahydro-1-1-dioxido-3-thienyl-amino-ethyl-es>

Generated by Cheméo on 2024-04-29 08:37:54.792470559 +0000 UTC m=+16669123.713047875.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.