

2-Thiazolidinethione

Other names:	Mercaptothiazoline Metabasal Thiazolidine-2-thione Thyroidan 1,3-Thiazolidine-2-thione 2(3H)-Thiazolethione, 4,5-dihydro- 2-Mercapto-«DELTA»2-thiazoline 2-Mercapto-2-thiazoline 2-Mercaptothiazoline 2-Thiazolidenethione 2-Thiazoline-2-thiol 2-Thiothiazolidone 4,5-Dihydro-2-mercaptothiazole Thiazolidin-2-thione Thiazoline-2-thiol 2-Thiozolidinethione Tetrahydrothiazole-2-thione 4,5-Dihydro-thiazole-2-thiol NSC 680 Sancelent 2MT WR 305
Inchi:	InChI=1S/C3H5NS2/c5-3-4-1-2-6-3/h1-2H2,(H,4,5)
InchiKey:	WGJCBBASTRWVJL-UHFFFAOYSA-N
Formula:	C3H5NS2
SMILES:	SC1=NCCS1
Mol. weight [g/mol]:	119.21
CAS:	96-53-7

Physical Properties

Property code	Value	Unit	Source
gf	225.00	kJ/mol	Joback Method
hf	176.59	kJ/mol	Joback Method
hfus	10.06	kJ/mol	Joback Method
hsub	100.50 ± 3.40	kJ/mol	NIST Webbook
hvap	42.55	kJ/mol	Joback Method
ie	8.25 ± 0.03	eV	NIST Webbook

ie	8.25	eV	NIST Webbook
log10ws	-1.08		Crippen Method
logp	1.019		Crippen Method
mcvol	80.650	ml/mol	McGowan Method
pc	6796.39	kPa	Joback Method
tb	456.52	K	Joback Method
tc	727.13	K	Joback Method
tf	343.44	K	Joback Method
vc	0.281	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.83	J/mol×K	682.02	Joback Method
cpg	144.07	J/mol×K	456.52	Joback Method
cpg	154.18	J/mol×K	501.62	Joback Method
cpg	163.60	J/mol×K	546.72	Joback Method
cpg	172.34	J/mol×K	591.82	Joback Method
cpg	180.41	J/mol×K	636.92	Joback Method
cpg	194.61	J/mol×K	727.13	Joback Method
hfust	16.80	kJ/mol	377.00	NIST Webbook
hsubt	99.80 ± 3.40	kJ/mol	342.00	NIST Webbook

Sources

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=C96537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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