Rhodanine

Other names:	2,4-Thiazolidinedione, 2-thio-
	2-Thio-4-ketothiazolidine
	2-Thioxo-4-thiazolidinone
	4-Oxo-2-thionothiazolidine
	4-Oxo-2-thiothiazolidin
	4-Oxo-2-thioxothiazoline
	4-Thiazolidinone, 2-thioxo-
	4-Thiazolidinone-2-thione
	NSC 1899
	Rhodanic acid
	Rhodanin
	Rhodaninic acid
	Rodanin
	USAF HA-2
Inchi:	InChI=1S/C3H3NOS2/c5-2-1-7-3(6)4-2/h1H2,(H,4,5,6)
InchiKey:	KIWUVOGUEXMXSV-UHFFFAOYSA-N
Formula:	C3H3NOS2
SMILES:	OC1=NC(=S)SC1
Mol. weight [g/mol]:	133.19
CAS:	141-84-4

Physical Properties

Property code	Value	Unit	Source
gf	149.64	kJ/mol	Joback Method
hf	100.98	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-1.77		Aqueous Solubility Prediction Method
log10ws	-1.77		Estimated Solubility Method
logp	0.975		Crippen Method
mcvol	82.220	ml/mol	McGowan Method
pc	7957.72	kPa	Joback Method
tb	558.48	K	Joback Method
tc	802.36	K	Joback Method
tf	442.65	K	Aqueous Solubility Prediction Method

vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.17	J/mol×K	558.48	Joback Method
cpg	168.35	J/mol×K	599.13	Joback Method
cpg	174.03	J/mol×K	639.77	Joback Method
cpg	179.24	J/mol×K	680.42	Joback Method
cpg	184.01	J/mol×K	721.06	Joback Method
cpg	188.38	J/mol×K	761.71	Joback Method
cpg	192.39	J/mol×K	802.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
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

tf: Normal melting (fusion) point

vc: Critical Volume