

2-Oxazolidinethione

Other names:	Carbamothioic acid, (2-hydroxyethyl)-, «gamma»-lactone Oxazolidine-2-thione 1,3-Oxazolidine-2-thione 2-Mercapto-2-oxazoline 2-Thiooxazolidone
Inchi:	InChI=1S/C3H5NOS/c6-3-4-1-2-5-3/h1-2H2,(H,4,6)
InchiKey:	UMURLIQHQSKULR-UHFFFAOYSA-N
Formula:	C3H5NOS
SMILES:	S=C1NCCO1
Mol. weight [g/mol]:	103.14
CAS:	5840-81-3

Physical Properties

Property code	Value	Unit	Source
gf	111.08	kJ/mol	Joback Method
hf	-3.52	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hsub	105.00 ± 4.40	kJ/mol	NIST Webbook
hvap	41.58	kJ/mol	Joback Method
ie	8.37	eV	NIST Webbook
ie	8.37 ± 0.03	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	-0.109		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
pc	6796.39	kPa	Joback Method
tb	436.13	K	Joback Method
tc	675.31	K	Joback Method
tf	333.98	K	Joback Method
vc	0.241	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.35	J/mol×K	635.44	Joback Method

cpg	121.58	J/mol×K	436.13	Joback Method
cpg	129.44	J/mol×K	475.99	Joback Method
cpg	136.70	J/mol×K	515.86	Joback Method
cpg	143.41	J/mol×K	555.72	Joback Method
cpg	149.62	J/mol×K	595.58	Joback Method
cpg	160.66	J/mol×K	675.31	Joback Method
hfust	15.90	kJ/mol	370.00	NIST Webbook
hsubt	104.30 ± 4.40	kJ/mol	339.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5840813&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
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
mcvol:	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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