2,4-Thiazolidinedione

Other names:	2,4-Dioxothiazolidine
	Thiazolidinedione
	Thiazolidinedione-2,4
	2,4(3H,5H)-Thiazoledione
	USAF ek-5496
	thiazolidine-2,4-dione
Inchi:	InChI=1S/C3H3NO2S/c5-2-1-7-3(6)4-2/h1H2,(H,4,5,6)
InchiKey:	ZOBPZXTWZATXDG-UHFFFAOYSA-N
Formula:	C3H3NO2S
SMILES:	O=C1N=C(O)CS1
Mol. weight [g/mol]:	117.13
CAS:	2295-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-63.80	kJ/mol	Joback Method
hf	-151.82	kJ/mol	Joback Method
hfus	9.62	kJ/mol	Joback Method
hvap	56.74	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.810		Crippen Method
mcvol	71.740	ml/mol	McGowan Method
pc	7561.44	kPa	Joback Method
tb	553.66	K	Joback Method
tc	793.69	K	Joback Method
tf	436.02	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.23	J/mol×K	553.66	Joback Method
cpg	163.99	J/mol×K	593.67	Joback Method
cpg	171.36	J/mol×K	633.67	Joback Method

cpg	178.31	J/mol×K	673.68	Joback Method
cpg	184.81	J/mol×K	713.68	Joback Method
cpg	190.82	J/mol×K	753.69	Joback Method
cpg	196.31	J/mol×K	793.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.20	K	2.50	NIST Webbook

Sources

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=C2295310&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume