

Thiodiglycolic anhydride

Other names:	1-Oxa-4-thia-cyclohexan-2,6-dione 1,4-Oxathiane-2,6-dione
Inchi:	InChI=1S/C4H4O3S/c5-3-1-8-2-4(6)7-3/h1-2H2
InchiKey:	RIIUAPMWDSRBSH-UHFFFAOYSA-N
Formula:	C4H4O3S
SMILES:	O=C1CSCC(=O)O1
Mol. weight [g/mol]:	132.14
CAS:	3261-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-276.48	kJ/mol	Joback Method
hf	-413.37	kJ/mol	Joback Method
hfus	7.54	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
log10ws	0.09		Crippen Method
logp	-0.197		Crippen Method
mvol	81.720	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
tb	525.56	K	Joback Method
tc	794.41	K	Joback Method
tf	392.92	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.85	J/molxK	525.56	Joback Method
cpg	179.52	J/molxK	570.37	Joback Method
cpg	189.77	J/molxK	615.18	Joback Method
cpg	199.50	J/molxK	659.99	Joback Method
cpg	208.64	J/molxK	704.80	Joback Method
cpg	217.11	J/molxK	749.60	Joback Method
cpg	224.82	J/molxK	794.41	Joback Method

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=C3261878&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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