Ethanol, 2,2'-thiobis-, diacetate

Other names:	Acetic acid, thiodiethylene ester
	Ethanol, 2,2'-thiodi-, diacetate
	2,2'-Thiodiethanol diacetate
	Bis(«beta»-thioethyl acetate)
	2,2'-thiodiethyl diacetate
Inchi:	InChI=1S/C8H14O4S/c1-7(9)11-3-5-13-6-4-12-8(2)10/h3-6H2,1-2H3
InchiKey:	HWLINJPYLXLANY-UHFFFAOYSA-N
Formula:	C8H14O4S
SMILES:	CC(=O)OCCSCCOC(C)=O
Mol. weight [g/mol]:	206.26
CAS:	4275-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-418.24	kJ/mol	Joback Method
hf	-656.18	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	58.53	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.846		Crippen Method
mcvol	154.810	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
tb	603.80	K	Joback Method
tc	804.36	K	Joback Method
tf	251.10 ± 0.60	K	NIST Webbook
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.17	J/mol×K	603.80	Joback Method
cpg	384.03	J/mol×K	637.23	Joback Method
cpg	395.33	J/mol×K	670.65	Joback Method
cpg	406.06	J/mol×K	704.08	Joback Method

cpg	416.21	J/mol×K	737.51	Joback Method
cpg	425.75	J/mol×K	770.94	Joback Method
cpg	434.68	J/mol×K	804.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4275289&Units=SI

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