Propionic acid, 3-mercapto-, ethylene ester

Other names: ethylene bis(3-mercaptopropionate)
Inchi: InChI=1S/C8H14O4S2/c9-7(1-5-13)11-3-4-12-8(10)2-6-14/h13-14H,1-6H2
InchiKey: HAQZWTGSNCDKTK-UHFFFAOYSA-N
Formula: C8H14O4S2
SMILES: O=C(CCS)OCCOC(=O)CCS
Mol. weight [g/mol]: 238.32
CAS: 22504-50-3

Physical Properties

Property code	Value	Unit	Source
gf	-392.58	kJ/mol	Joback Method
hf	-621.09	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.713		Crippen Method
mcvol	171.160	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	660.74	K	Joback Method
tc	877.89	K	Joback Method
tf	397.16	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.06	J/mol×K	660.74	Joback Method
cpg	427.78	J/mol×K	696.93	Joback Method
cpg	438.81	J/mol×K	733.12	Joback Method
cpg	449.14	J/mol×K	769.32	Joback Method
cpg	458.75	J/mol×K	805.51	Joback Method
cpg	467.64	J/mol×K	841.70	Joback Method
cpg	475.81	J/mol×K	877.89	Joback Method

Sources

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=C22504503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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