1,1-Diethoxy-1-(ethylthio)ethane

Inchi: InChI=1S/C8H18O2S/c1-5-9-8(4,10-6-2)11-7-3/h5-7H2,1-4H3
InchiKey: DITBNWASEYIFQA-UHFFFAOYSA-N
Formula: C8H18O2S
SMILES: CCOC(C)(OCC)SCC
Mol. weight [g/mol]: 178.29
CAS: 68058-53-7

Physical Properties

Property code	Value	Unit	Source
gf	-157.56	kJ/mol	Joback Method
hf	-454.00 ± 17.00	kJ/mol	NIST Webbook
hfus	15.57	kJ/mol	Joback Method
hvap	43.74	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.486		Crippen Method
mcvol	151.670	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	492.83	K	Joback Method
tc	688.13	K	Joback Method
tf	261.20	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.42	J/mol×K	492.83	Joback Method
cpg	353.92	J/mol×K	525.38	Joback Method
cpg	367.79	J/mol×K	557.93	Joback Method
cpg	381.06	J/mol×K	590.48	Joback Method
cpg	393.71	J/mol×K	623.03	Joback Method
cpg	405.76	J/mol×K	655.58	Joback Method
cpg	417.21	J/mol×K	688.13	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=C68058537&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