2,4,6-Triethyl-[1,3,5]dioxathiane, stereoisomer 1

Inchi: InChI=1S/C9H18O2S/c1-4-7-10-8(5-2)12-9(6-3)11-7/h7-9H,4-6H2,1-3H3
InchiKey: SVNXDVGQOSCMJR-UHFFFAOYSA-N
Formula: C9H18O2S
SMILES: CCC1OC(CC)SC(CC)O1
Mol. weight [g/mol]: 190.30

Physical Properties

Property code	Value	Unit	Source
gf	-98.45	kJ/mol	Joback Method
hf	-434.19	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	50.27	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.975		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
ripol	1550.00		NIST Webbook
ripol	1550.00		NIST Webbook
tb	517.26	K	Joback Method
tc	727.59	K	Joback Method
tf	326.68	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.17	J/mol×K	517.26	Joback Method
cpg	391.21	J/mol×K	552.32	Joback Method
cpg	408.36	J/mol×K	587.37	Joback Method
cpg	424.64	J/mol×K	622.43	Joback Method
cpg	440.06	J/mol×K	657.48	Joback Method
cpg	454.62	J/mol×K	692.54	Joback Method
cpg	468.34	J/mol×K	727.59	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=R495008&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume