s-Trioxane, 2,4,6-triethyl-

Other names: Parapropionaldehyde
2,4,6-Triethyl-s-trioxane
1,3,5-Trioxane, 2,4,6-triethyl-
2,4,6-Triethyl-[1,3,5]trioxane, stereoisomer 2
Inchi: InChI=1S/C9H18O3/c1-4-7-10-8(5-2)12-9(6-3)11-7/h7-9H,4-6H2,1-3H3
InchiKey: GYBGKXFOKOSPLS-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCC1OC(CC)OC(CC)O1
Mol. weight [g/mol]: 174.24
CAS: 2396-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-224.43	kJ/mol	Joback Method
hf	-611.45	kJ/mol	Joback Method
hfus	36.98	kJ/mol	Joback Method
hvap	48.97	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.258		Crippen Method
mcvol	144.420	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
ripol	1285.00		NIST Webbook
ripol	1285.00		NIST Webbook
tb	496.38	K	Joback Method
tc	693.27	K	Joback Method
tf	269.80	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.76	J/mol×K	496.38	Joback Method
cpg	434.51	J/mol×K	660.45	Joback Method
cpg	420.08	J/mol×K	627.64	Joback Method

cpg	404.89	J/mol×K	594.82	Joback Method
cpg	388.95	J/mol×K	562.01	Joback Method
cpg	372.24	J/mol×K	529.19	Joback Method
cpg	448.18	J/mol×K	693.27	Joback Method
dvisc	0.0003543	Pa×s	496.38	Joback Method
dvisc	0.0004519	Pa×s	458.62	Joback Method
dvisc	0.0006022	Pa×s	420.85	Joback Method
dvisc	0.0008492	Pa×s	383.09	Joback Method
dvisc	0.0012910	Pa×s	345.33	Joback Method
dvisc	0.0021753	Pa×s	307.56	Joback Method
dvisc	0.0042417	Pa×s	269.80	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=C2396421&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
dvisc: Dynamic viscosity
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