

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

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

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	1254.00		NIST Webbook
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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/molxK	496.38	Joback Method
cpg	372.24	J/molxK	529.19	Joback Method
cpg	388.95	J/molxK	562.01	Joback Method
cpg	404.89	J/molxK	594.82	Joback Method
cpg	420.08	J/molxK	627.64	Joback Method
cpg	434.51	J/molxK	660.45	Joback Method
cpg	448.18	J/molxK	693.27	Joback Method
dvisc	0.0042417	Paxs	269.80	Joback Method

dvisc	0.0021753	Paxs	307.56	Joback Method
dvisc	0.0012910	Paxs	345.33	Joback Method
dvisc	0.0008492	Paxs	383.09	Joback Method
dvisc	0.0006022	Paxs	420.85	Joback Method
dvisc	0.0004519	Paxs	458.62	Joback Method
dvisc	0.0003543	Paxs	496.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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