1,3,5-Trioxane, 2,4,6-tripropyl-

Other names:	s-Trioxane, 2,4,6-tripropyl-
	Parabutyraldehyde
	2,4,6-Tripropyl-s-trioxane
	p-n-Butyraldehyde
	2,4,6-tripropyl-1,3,5-trioxane
Inchi:	InChI=1S/C12H24O3/c1-4-7-10-13-11(8-5-2)15-12(14-10)9-6-3/h10-12H,4-9H2,1-3H3
InchiKey:	OXSRKPVVVMMMER-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CCCC1OC(CCC)OC(CCC)O1
Mol. weight [g/mol]:	216.32
CAS:	2396-43-2

Physical Properties

Property code	Value	Unit	Source
gf	-199.17	kJ/mol	Joback Method
hf	-673.37	kJ/mol	Joback Method
hfus	44.75	kJ/mol	Joback Method
hvap	55.65	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.428		Crippen Method
mcvol	186.690	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
tb	565.02	K	Joback Method
tc	754.58	K	Joback Method
tf	303.61	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.09	J/mol×K	565.02	Joback Method
cpg	591.43	J/mol×K	722.98	Joback Method
cpg	575.53	J/mol×K	691.39	Joback Method
cpg	558.75	J/mol×K	659.80	Joback Method

cpg	541.09	J/mol×K	628.21	Joback Method
cpg	522.54	J/mol×K	596.61	Joback Method
cpg	606.48	J/mol×K	754.58	Joback Method
dvisc	0.0002787	Pa×s	565.02	Joback Method
dvisc	0.0003611	Pa×s	521.45	Joback Method
dvisc	0.0004903	Pa×s	477.88	Joback Method
dvisc	0.0007079	Pa×s	434.31	Joback Method
dvisc	0.0011093	Pa×s	390.75	Joback Method
dvisc	0.0019460	Pa×s	347.18	Joback Method
dvisc	0.0040110	Pa×s	303.61	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=C2396432&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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