Pentane, 1,1,1-trimethoxy-

Other names:	Orthovaleric acid, trimethyl ester
	Trimethyl orthovalerate
	1,1,1-Trimethoxypentane
	ortho-n-Valeric acid trimethyl ester
Inchi:	InChI=1S/C8H18O3/c1-5-6-7-8(9-2,10-3)11-4/h5-7H2,1-4H3
InchiKey:	XUXVVQKJULMMKX-UHFFFAOYSA-N
Formula:	C8H18O3
SMILES:	CCCCC(OC)(OC)OC
Mol. weight [g/mol]:	162.23
CAS:	13820-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-295.68	kJ/mol	Joback Method
hf	-613.86	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	39.34	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.770		Crippen Method
mcvol	141.190	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	438.20	K	NIST Webbook
tc	620.72	K	Joback Method
tf	249.03	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.58	J/mol×K	446.47	Joback Method
cpg	323.05	J/mol×K	475.51	Joback Method
cpg	336.08	J/mol×K	504.55	Joback Method
cpg	348.67	J/mol×K	533.60	Joback Method
cpg	360.82	J/mol×K	562.64	Joback Method

cpg	372.51	J/mol×K	591.68	Joback Method
cpg	383.76	J/mol×K	620.72	Joback Method
dvisc	0.0032508	Pa×s	249.03	Joback Method
dvisc	0.0014858	Pa×s	281.94	Joback Method
dvisc	0.0007999	Pa×s	314.84	Joback Method
dvisc	0.0004841	Pa×s	347.75	Joback Method
dvisc	0.0003196	Pa×s	380.66	Joback Method
dvisc	0.0002254	Pa×s	413.56	Joback Method
dvisc	0.0001674	Pa×s	446.47	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=C13820092&Units=SI

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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