Trimethyl orthobutyrate

Other names:	ortho-n-Butyric acid trimethyl ester
	Butane, 1,1,1-trimethoxy-
	1,1,1-trimethoxybutane
Inchi:	InChI=1S/C7H16O3/c1-5-6-7(8-2,9-3)10-4/h5-6H2,1-4H3
InchiKey:	JAFMOTJMRSZOJE-UHFFFAOYSA-N
Formula:	C7H16O3
SMILES:	CCCC(OC)(OC)OC
Mol. weight [g/mol]:	148.20
CAS:	43083-12-1

Physical Properties

Property code	Value	Unit	Source
gf	-304.10	kJ/mol	Joback Method
hf	-593.22	kJ/mol	Joback Method
hfus	10.04	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.380		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	419.20	K	NIST Webbook
tc	599.04	K	Joback Method
tf	237.76	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.18	J/mol×K	423.59	Joback Method
cpg	280.51	J/mol×K	452.83	Joback Method
cpg	292.46	J/mol×K	482.07	Joback Method
cpg	304.02	J/mol×K	511.32	Joback Method
cpg	315.20	J/mol×K	540.56	Joback Method
cpg	325.98	J/mol×K	569.80	Joback Method

cpg	336.37	J/mol×K	599.04	Joback Method
dvisc	0.0033515	Pa×s	237.76	Joback Method
dvisc	0.0015609	Pa×s	268.73	Joback Method
dvisc	0.0008514	Pa×s	299.70	Joback Method
dvisc	0.0005202	Pa×s	330.67	Joback Method
dvisc	0.0003458	Pa×s	361.65	Joback Method
dvisc	0.0002452	Pa×s	392.62	Joback Method
dvisc	0.0001828	Pa×s	423.59	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C43083121&Units=SI
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

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