Butane, 1,1,3-trimethoxy-

Other names:	Butyraldehyde, 3-methoxy-, dimethyl acetal
	1,1,3-Trimethoxybutane
	3-Methoxybutyraldehyde dimethyl acetal
Inchi:	InChI=1S/C7H16O3/c1-6(8-2)5-7(9-3)10-4/h6-7H,5H2,1-4H3
InchiKey:	OMAKZNALRADTRX-UHFFFAOYSA-N
Formula:	C7H16O3
SMILES:	COC(C)CC(OC)OC
Mol. weight [g/mol]:	148.20
CAS:	10138-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-311.82	kJ/mol	Joback Method
hf	-595.03	kJ/mol	Joback Method
hfus	10.40	kJ/mol	Joback Method
hvap	37.63	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	1.030		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	888.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	430.20	K	NIST Webbook
tc	598.37	K	Joback Method
tf	205.34	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.11	J/mol×K	425.94	Joback Method
cpg	277.89	J/mol×K	454.68	Joback Method
cpg	289.41	J/mol×K	483.42	Joback Method

cpg	300.66	J/mol×K	512.16	Joback Method
cpg	311.63	J/mol×K	540.90	Joback Method
cpg	322.29	J/mol×K	569.63	Joback Method
cpg	332.64	J/mol×K	598.37	Joback Method
dvisc	0.0055798	Pa×s	205.34	Joback Method
dvisc	0.0019646	Pa×s	242.11	Joback Method
dvisc	0.0009109	Pa×s	278.87	Joback Method
dvisc	0.0005052	Pa×s	315.64	Joback Method
dvisc	0.0003168	Pa×s	352.41	Joback Method
dvisc	0.0002170	Pa×s	389.17	Joback Method
dvisc	0.0001587	Pa×s	425.94	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=C10138893&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume