

1,3,3-Trimethoxybutane

Other names:	Butane, 1,3,3-trimethoxy- 4-methoxybutan-2-one-dimethylacetal
Inchi:	InChI=1S/C7H16O3/c1-7(9-3,10-4)5-6-8-2/h5-6H2,1-4H3
InchiKey:	DIQSNTFKLAYVOT-UHFFFAOYSA-N
Formula:	C7H16O3
SMILES:	COCCC(C)(OC)OC
Mol. weight [g/mol]:	148.20
CAS:	6607-66-5

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	-0.62		Crippen Method
logp	1.032		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	423.59	K	Joback Method
tc	599.04	K	Joback Method
tf	237.76	K	Joback Method
vc	0.470	m ³ /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	Paxs	237.76	Joback Method
dvisc	0.0015609	Paxs	268.73	Joback Method
dvisc	0.0008514	Paxs	299.70	Joback Method
dvisc	0.0005202	Paxs	330.67	Joback Method
dvisc	0.0003458	Paxs	361.65	Joback Method
dvisc	0.0002452	Paxs	392.62	Joback Method
dvisc	0.0001828	Paxs	423.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	2.70	NIST Webbook

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=C6607665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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