1,3,3-TRIMETHOXYBUTANE

Other names: 4-methoxybutan-2-one-dimethylacetal
Butane, 1,3,3-trimethoxy-
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

Physical Properties

Property code	Value	Unit	Source
af	0.4236		Cheméo Relay (1.0)
hf	-589.66	kJ/mol	Cheméo Relay (1.0)
hfus	10.04	kJ/mol	Joback Method
ie	9.24	eV	Cheméo Relay (1.0)
logp	1.032		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	428.70	K	Cheméo Relay (1.0)
tc	597.84	K	Cheméo Relay (1.0)
tf	211.29	K	Cheméo Relay (1.0)
vc	0.464	m3/kmol	Cheméo Relay (1.0)

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

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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6607665&Units=SI

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
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