

1,1,1-Trimethoxy-2-methylpropane

Inchi:	InChI=1S/C7H16O3/c1-6(2)7(8-3,9-4)10-5/h6H,1-5H3
InchiKey:	BGLARIMANCDMQX-UHFFFAOYSA-N
Formula:	C7H16O3
SMILES:	COC(OC)(OC)C(C)C
Mol. weight [g/mol]:	148.20
CAS:	52698-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-306.54	kJ/mol	Joback Method
hf	-598.50	kJ/mol	Joback Method
hfus	6.51	kJ/mol	Joback Method
hvap	44.10 ± 4.20	kJ/mol	NIST Webbook
log10ws	-0.87		Crippen Method
logp	1.235		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	423.15	K	Joback Method
tc	602.59	K	Joback Method
tf	222.76	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.20	J/mol×K	423.15	Joback Method
cpg	280.90	J/mol×K	453.06	Joback Method
cpg	293.19	J/mol×K	482.96	Joback Method
cpg	305.07	J/mol×K	512.87	Joback Method
cpg	316.54	J/mol×K	542.77	Joback Method
cpg	327.59	J/mol×K	572.68	Joback Method
cpg	338.22	J/mol×K	602.59	Joback Method
dvisc	0.0054284	Paxs	222.76	Joback Method
dvisc	0.0021104	Paxs	256.16	Joback Method

dvisc	0.0010202	Paxs	289.56	Joback Method
dvisc	0.0005732	Paxs	322.95	Joback Method
dvisc	0.0003588	Paxs	356.35	Joback Method
dvisc	0.0002434	Paxs	389.75	Joback Method
dvisc	0.0001755	Paxs	423.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C52698461&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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