

1,1,1-Trimethoxy-2-methylbutane

Inchi:	InChI=1S/C8H18O3/c1-6-7(2)8(9-3,10-4)11-5/h7H,6H2,1-5H3
InchiKey:	QWPCHBGGMCMXPS-UHFFFAOYSA-N
Formula:	C8H18O3
SMILES:	CCC(C)C(OC)(OC)OC
Mol. weight [g/mol]:	162.23
CAS:	98944-42-4

Physical Properties

Property code	Value	Unit	Source
gf	-298.12	kJ/mol	Joback Method
hf	-619.14	kJ/mol	Joback Method
hfus	9.10	kJ/mol	Joback Method
hvap	38.95	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.626		Crippen Method
mcvol	141.190	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	446.03	K	Joback Method
tc	624.11	K	Joback Method
tf	234.03	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.65	J/molxK	446.03	Joback Method
cpg	323.50	J/molxK	475.71	Joback Method
cpg	336.88	J/molxK	505.39	Joback Method
cpg	349.79	J/molxK	535.07	Joback Method
cpg	362.23	J/molxK	564.75	Joback Method
cpg	374.20	J/molxK	594.43	Joback Method
cpg	385.69	J/molxK	624.11	Joback Method
dvisc	0.0051370	Paxs	234.03	Joback Method
dvisc	0.0019718	Paxs	269.36	Joback Method

dvisc	0.0009451	Paxs	304.70	Joback Method
dvisc	0.0005278	Paxs	340.03	Joback Method
dvisc	0.0003289	Paxs	375.36	Joback Method
dvisc	0.0002223	Paxs	410.70	Joback Method
dvisc	0.0001599	Paxs	446.03	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=C98944424&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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