

1,1,1-Trimethoxy-3-methylbutane

Inchi:	InChI=1S/C8H18O3/c1-7(2)6-8(9-3,10-4)11-5/h7H,6H2,1-5H3
InchiKey:	WMHIOPJVXYRZFG-UHFFFAOYSA-N
Formula:	C8H18O3
SMILES:	COC(CC(C)C)(OC)OC
Mol. weight [g/mol]:	162.23
CAS:	74252-65-6

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/mol×K	446.03	Joback Method
cpg	374.20	J/mol×K	594.43	Joback Method
cpg	362.23	J/mol×K	564.75	Joback Method
cpg	349.79	J/mol×K	535.07	Joback Method
cpg	336.88	J/mol×K	505.39	Joback Method
cpg	323.50	J/mol×K	475.71	Joback Method
cpg	385.69	J/mol×K	624.11	Joback Method
dvisc	0.0001599	Pa×s	446.03	Joback Method
dvisc	0.0002223	Pa×s	410.70	Joback Method

dvisc	0.0003289	Pa×s	375.36	Joback Method
dvisc	0.0005278	Pa×s	340.03	Joback Method
dvisc	0.0009451	Pa×s	304.70	Joback Method
dvisc	0.0019718	Pa×s	269.36	Joback Method
dvisc	0.0051370	Pa×s	234.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74252656&Units=SI
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

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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