

1-Propene, 1,3,3-trimethoxy-

Other names:	Acrolein, 3-methoxy-, dimethyl acetal 1,3,3-Trimethoxy-1-propene 1,3,3-Trimethoxypropene 1,3,3-Trimethoxy-2-propene
Inchi:	InChI=1S/C6H12O3/c1-7-5-4-6(8-2)9-3/h4-6H,1-3H3/b5-4+
InchiKey:	JGVSIZVWGGQMPY-SNAWJCMRSA-N
Formula:	C6H12O3
SMILES:	COC=CC(OC)OC
Mol. weight [g/mol]:	132.16
CAS:	17576-35-1

Physical Properties

Property code	Value	Unit	Source
gf	-237.58	kJ/mol	Joback Method
hf	-451.89	kJ/mol	Joback Method
hfus	11.54	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.765		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	407.66	K	Joback Method
tc	585.73	K	Joback Method
tf	203.99	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.99	J/mol×K	407.66	Joback Method
cpg	258.79	J/mol×K	556.06	Joback Method
cpg	249.93	J/mol×K	526.38	Joback Method
cpg	240.81	J/mol×K	496.70	Joback Method
cpg	231.44	J/mol×K	467.02	Joback Method

cpg	221.83	J/mol×K	437.34	Joback Method
cpg	267.38	J/mol×K	585.73	Joback Method
dvisc	0.0001434	Pa×s	407.66	Joback Method
dvisc	0.0001897	Pa×s	373.71	Joback Method
dvisc	0.0002654	Pa×s	339.77	Joback Method
dvisc	0.0004000	Pa×s	305.82	Joback Method
dvisc	0.0006679	Pa×s	271.88	Joback Method
dvisc	0.0012910	Pa×s	237.94	Joback Method
dvisc	0.0031068	Pa×s	203.99	Joback Method

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=C17576351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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