2-Butene, 1,1-dimethoxy-

Other names: Crotonaldehyde, dimethyl acetal
2-Butenal dimethyl acetal
1,1-dimethoxybut-2-ene
Inchi: InChI=1S/C6H12O2/c1-4-5-6(7-2)8-3/h4-6H,1-3H3/b5-4+
InchiKey: NOYRGONWBIVLEL-SNAWJCMRSA-N
Formula: C6H12O2
SMILES: CC=CC(OC)OC
Mol. weight [g/mol]: 116.16
CAS: 21962-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-132.58	kJ/mol	Joback Method
hf	-303.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-346.00 ± 2.00	kJ/mol	NIST Webbook
hfus	10.35	kJ/mol	Joback Method
hvap	43.26	kJ/mol	NIST Webbook
hvap	43.00	kJ/mol	NIST Webbook
log10ws	-0.97		Crippen Method
logp	1.181		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	385.24	K	Joback Method
tc	563.20	K	Joback Method
tf	181.76	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.91	J/mol×K	385.24	Joback Method
cpg	199.94	J/mol×K	414.90	Joback Method
cpg	209.66	J/mol×K	444.56	Joback Method
cpg	219.09	J/mol×K	474.22	Joback Method

cpg	228.21	J/mol×K	503.88	Joback Method
cpg	237.04	J/mol×K	533.54	Joback Method
cpg	245.56	J/mol×K	563.20	Joback Method
dvisc	0.0043568	Pa×s	181.76	Joback Method
dvisc	0.0016340	Pa×s	215.67	Joback Method
dvisc	0.0007999	Pa×s	249.59	Joback Method
dvisc	0.0004646	Pa×s	283.50	Joback Method
dvisc	0.0003031	Pa×s	317.41	Joback Method
dvisc	0.0002147	Pa×s	351.33	Joback Method
dvisc	0.0001616	Pa×s	385.24	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=C21962243&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
hfl:	Liquid phase 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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