2-Butene, 1,4-dimethoxy-

Other names: 1,4-Dimethoxy-2-butene
2-Butene-1,4-diol, dimethyl ether
(2E)-1,4-Dimethoxy-2-butene
Inchi: InChI=1S/C6H12O2/c1-7-5-3-4-6-8-2/h3-4H,5-6H2,1-2H3/b4-3+
InchiKey: RXNMLQHZBCJMBA-ONEGZZNKSA-N
Formula: C6H12O2
SMILES: COCC=CCOC
Mol. weight [g/mol]: 116.16
CAS: 26649-86-5

Physical Properties

Property code	Value	Unit	Source
gf	-130.14	kJ/mol	Joback Method
hf	-314.39	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	33.73	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	0.835		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	884.20		NIST Webbook
rinpol	884.20		NIST Webbook
tb	385.68	K	Joback Method
tc	559.54	K	Joback Method
tf	196.76	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.97	J/mol×K	385.68	Joback Method
cpg	199.67	J/mol×K	414.66	Joback Method
cpg	209.09	J/mol×K	443.63	Joback Method
cpg	218.24	J/mol×K	472.61	Joback Method

cpg	227.10	J/mol×K	501.58	Joback Method
cpg	235.68	J/mol×K	530.56	Joback Method
cpg	243.98	J/mol×K	559.54	Joback Method
dvisc	0.0025550	Pa×s	196.76	Joback Method
dvisc	0.0011850	Pa×s	228.25	Joback Method
dvisc	0.0006622	Pa×s	259.73	Joback Method
dvisc	0.0004196	Pa×s	291.22	Joback Method
dvisc	0.0002907	Pa×s	322.71	Joback Method
dvisc	0.0002149	Pa×s	354.19	Joback Method
dvisc	0.0001670	Pa×s	385.68	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26649865&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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