

2-BUTENE, 1,4-DIMETHOXY-

Other names:	(2E)-1,4-Dimethoxy-2-butene 1,4-Dimethoxy-2-butene 2-Butene-1,4-diol, dimethyl ether
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:	COC/C=C/COC
Mol. weight [g/mol]:	116.16

Physical Properties

Property code	Value	Unit	Source
hfus	13.87	kJ/mol	Joback Method
ie	9.03	eV	Cheméo Relay (1.0)
logp	0.835		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
rinpol	884.20		NIST Webbook
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tb	416.24	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26649865&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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