

Ethane, 1,1-dimethoxy-

Other names:	Acetaldehyde, dimethyl acetal Dimethyl acetal Ethylidene dimethyl ether 1,1-Dimethoxyethane CH ₃ CH(OCH ₃) ₂ Dimethyl aldehyde UN 2377 3-Methyl-2,4-dioxapentane Acetaldehyde methyl acetal
Inchi:	InChI=1S/C4H10O2/c1-4(5-2)6-3/h4H,1-3H3
InchiKey:	SPEUIVXLLWOEMJ-UHFFFAOYSA-N
Formula:	C ₄ H ₁₀ O ₂
SMILES:	COC(C)OC
Mol. weight [g/mol]:	90.12
CAS:	534-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-229.64	kJ/mol	Joback Method
hf	-395.61	kJ/mol	Joback Method
hfus	4.97	kJ/mol	Joback Method
hvap	36.40 ± 0.10	kJ/mol	NIST Webbook
ie	10.00 ± 10.00	eV	NIST Webbook
log10ws	-0.28		Crippen Method
logp	0.625		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	588.00		NIST Webbook
rinpol	547.00		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	547.00		NIST Webbook
rinpol	588.00		NIST Webbook
tb	334.45 ± 0.50	K	NIST Webbook
tb	336.00 ± 2.00	K	NIST Webbook
tb	337.70	K	NIST Webbook

tc	504.58	K	Joback Method
tf	164.30	K	Joback Method
vc	0.289	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.35	J/mol×K	504.58	Joback Method
cpg	171.73	J/mol×K	476.37	Joback Method
cpg	164.99	J/mol×K	448.16	Joback Method
cpg	158.12	J/mol×K	419.95	Joback Method
cpg	151.14	J/mol×K	391.74	Joback Method
cpg	144.07	J/mol×K	363.53	Joback Method
cpg	136.91	J/mol×K	335.32	Joback Method
dvisc	0.0039085	Paxs	164.30	Joback Method
dvisc	0.0001930	Paxs	335.32	Joback Method
dvisc	0.0002524	Paxs	306.82	Joback Method
dvisc	0.0003489	Paxs	278.31	Joback Method
dvisc	0.0005190	Paxs	249.81	Joback Method
dvisc	0.0008554	Paxs	221.31	Joback Method
dvisc	0.0016342	Paxs	192.80	Joback Method
hvapt	33.40	kJ/mol	303.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C534156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h vap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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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