

Ethene, methoxy-

Other names:	1-Methoxyethylene CH2=CHOCH3 Ether, methyl vinyl METHOXYETHYLENE Methoxyethene Methyl vinyl ether UN 1087 VINYL METHYL ETHER
Inchi:	InChI=1S/C3H6O/c1-3-4-2/h3H,1H2,2H3
InchiKey:	XJRBAMWJDBPFIM-UHFFFAOYSA-N
Formula:	C3H6O
SMILES:	C=COC
Mol. weight [g/mol]:	58.08
CAS:	107-25-5

Physical Properties

Property code	Value	Unit	Source
af	0.3400		KDB
affp	859.20	kJ/mol	NIST Webbook
basg	830.30	kJ/mol	NIST Webbook
gf	-42.78	kJ/mol	Joback Method
hf	-112.04	kJ/mol	Joback Method
hfus	3.43	kJ/mol	Joback Method
hvap	24.01	kJ/mol	Joback Method
ie	9.05	eV	NIST Webbook
ie	8.95 ± 0.01	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	8.93 ± 0.02	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
log10ws	-0.51		Crippen Method
logp	0.776		Crippen Method
mcvol	54.700	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4760.00	kPa	KDB
rinpol	416.00		NIST Webbook

rinpol	416.00		NIST Webbook
tb	278.70	K	NIST Webbook
tb	278.15	K	NIST Webbook
tb	278.00	K	KDB
tc	436.00	K	KDB
tf	151.55	K	NIST Webbook
tf	151.50	K	KDB
vc	0.205	m3/kmol	KDB
zc	0.2691770		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.83	J/mol×K	425.19	Joback Method
cpg	95.50	J/mol×K	397.58	Joback Method
cpg	91.07	J/mol×K	369.97	Joback Method
cpg	86.54	J/mol×K	342.36	Joback Method
cpg	81.90	J/mol×K	314.75	Joback Method
cpg	77.18	J/mol×K	287.14	Joback Method
cpg	104.06	J/mol×K	452.81	Joback Method
dvisc	0.0014817	Pa×s	144.04	Joback Method
dvisc	0.0001564	Pa×s	287.14	Joback Method
dvisc	0.0001920	Pa×s	263.29	Joback Method
dvisc	0.0002455	Pa×s	239.44	Joback Method
dvisc	0.0003315	Pa×s	215.59	Joback Method
dvisc	0.0004823	Pa×s	191.74	Joback Method
dvisc	0.0007806	Pa×s	167.89	Joback Method
hvapt	23.40	kJ/mol	345.00	NIST Webbook
rhoI	750.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62224e+01
Coeff. B	-3.71356e+03
Coeff. C	4.13240e+01

Temperature range (K), min.	191.72
Temperature range (K), max.	299.03

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.24206e+01
Coeff. B	-4.92509e+03
Coeff. C	-7.20457e+00
Coeff. D	5.46059e-06
Temperature range (K), min.	151.15
Temperature range (K), max.	437.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol997.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107255&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=997
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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