Benzene, (ethoxymethyl)-

Other names:	(ETHOXYMETHYL)BENZENE
	BENZYL ETHYL OXIDE
	Benzyl ethyl ether
	Ether, benzyl ethyl
	Ethyl benzyl ether
Inchi:	InChI=1S/C9H12O/c1-2-10-8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	AXPZDYVDTMMLNB-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCOCc1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	539-30-0

Physical Properties

Property code	Value	Unit	Source
gf	32.31	kJ/mol	Joback Method
hf	-124.78	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	53.50 ± 0.40	kJ/mol	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.223		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1039.50		NIST Webbook
rinpol	1047.90		NIST Webbook
rinpol	1046.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1439.00		NIST Webbook
tb	458.20	K	NIST Webbook
tb	462.00	K	NIST Webbook

tb	458.20 ± 0.60	K	NIST Webbook
tb	458.35 ± 0.40	K	NIST Webbook
tc	660.22	K	Joback Method
tf	239.84	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.41	J/mol×K	660.22	Joback Method
cpg	238.54	J/mol×K	454.42	Joback Method
cpg	252.16	J/mol×K	488.72	Joback Method
cpg	265.10	J/mol×K	523.02	Joback Method
cpg	277.38	J/mol×K	557.32	Joback Method
cpg	289.01	J/mol×K	591.62	Joback Method
cpg	300.02	J/mol×K	625.92	Joback Method
dvisc	0.0002037	Pa×s	454.42	Joback Method
dvisc	0.0027046	Pa×s	239.84	Joback Method
dvisc	0.0013289	Pa×s	275.60	Joback Method
dvisc	0.0007687	Pa×s	311.37	Joback Method
dvisc	0.0004978	Pa×s	347.13	Joback Method
dvisc	0.0003496	Pa×s	382.89	Joback Method
dvisc	0.0002608	Pa×s	418.66	Joback Method
hvapt	48.00	kJ/mol	379.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.00	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.50689e+01
Coeff. B	-4.34681e+03
Coeff. C	-4.22100e+01
Temperature range (K), min.	336.28
Temperature range (K), max.	487.70

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.98020e+01
Coeff. B	-7.77928e+03
Coeff. C	-6.31706e+00
Coeff. D	2.34148e-06
Temperature range (K), min.	275.65
Temperature range (K), max.	662.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1029.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C539300&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1029

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

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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume