2-ISOBUTOXYETHANOL

Other names:	2-(2-methylpropoxy)ethanol
	Ektasolve eib
	Ethanol, 2-(2-methylpropoxy)-
	Ethanol, 2-isobutoxy-
	ethylene glycol monoisobutyl ether
	isobutyl cellosolve
Inchi:	InChI=1S/C6H14O2/c1-6(2)5-8-4-3-7/h6-7H,3-5H2,1-2H3
InchiKey:	HHAPGMVKBLELOE-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(C)COCCO
Mol. weight [g/mol]:	118.18
CAS:	4439-24-1

Physical Properties

Property code	Value	Unit	Source
hf	-463.65	kJ/mol	Cheméo Relay (1.0)
hfus	13.05	kJ/mol	Joback Method
hvap	51.34	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-0.24		Cheméo Relay (1.0)
logp	0.651		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	927.00		NIST Webbook
rinpol	878.00		NIST Webbook
ripol	1400.00		NIST Webbook
tb	433.15	K	NIST Webbook
tc	624.76	K	Cheméo Relay (1.0)
tf	195.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.39	J/mol×K	588.02	Joback Method

cpg	283.50	J/mol×K	615.45	Joback Method
cpg	239.95	J/mol×K	478.28	Joback Method
cpg	249.26	J/mol×K	505.71	Joback Method
cpg	258.28	J/mol×K	533.15	Joback Method
cpg	266.99	J/mol×K	560.58	Joback Method
cpg	230.32	J/mol×K	450.84	Joback Method
dvisc	0.0038675	Pa×s	300.57	Joback Method
dvisc	0.0143235	Pa×s	263.00	Joback Method
dvisc	0.0820702	Pa×s	225.43	Joback Method
dvisc	0.0013969	Pa×s	338.13	Joback Method
dvisc	0.0006185	Pa×s	375.70	Joback Method
dvisc	0.0003176	Pa×s	413.27	Joback Method
dvisc	0.0001822	Pa×s	450.84	Joback Method
hvapt	48.10	kJ/mol	388.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62951e+01
Coeff. B	-4.33890e+03
Coeff. C	-6.15660e+01
Temperature range (K), min.	332.62
Temperature range (K), max.	456.60

Sources

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

Group-contribution to limiting partial molar isentropic compressions of small amphiphile molecules in water. The temperature effect: https://www.doi.org/10.1016/j.jct.2013.10.013

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

A (vapor + liquid) equilibria of the {carbon dioxide + isopropoxyethanol (iOSE1)} and the {carbon dioxide + isobutoxyethanol (iC4E1)} systems: https://www.doi.org/10.1016/j.jct.2007.06.005

Cheméo Relay (1.0):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4439241&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point