

Propane, 1-(1-ethoxyethoxy)-

Other names:	Acetaldehyde, ethyl propyl acetal 1-Ethoxy-1-propoxyethane 1-(1-Ethoxyethoxy)propane Ethane, 1-ethoxy-1-propoxy
Inchi:	InChI=1S/C7H16O2/c1-4-6-9-7(3)8-5-2/h7H,4-6H2,1-3H3
InchiKey:	XKPTXCDASJWOLK-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCCOC(C)OCC
Mol. weight [g/mol]:	132.20
CAS:	20680-10-8

Physical Properties

Property code	Value	Unit	Source
gf	-204.38	kJ/mol	Joback Method
hf	-457.53	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	35.61	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.796		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	821.00		NIST Webbook
tb	403.96	K	Joback Method
tc	572.52	K	Joback Method
tf	198.11	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.30	J/molxK	403.96	Joback Method
cpg	253.90	J/molxK	432.05	Joback Method
cpg	265.20	J/molxK	460.15	Joback Method
cpg	276.21	J/molxK	488.24	Joback Method

cpg	286.90	J/mol×K	516.33	Joback Method
cpg	297.29	J/mol×K	544.43	Joback Method
cpg	307.36	J/mol×K	572.52	Joback Method
dvisc	0.0047999	Paxs	198.11	Joback Method
dvisc	0.0018890	Paxs	232.42	Joback Method
dvisc	0.0009450	Paxs	266.73	Joback Method
dvisc	0.0005536	Paxs	301.04	Joback Method
dvisc	0.0003618	Paxs	335.34	Joback Method
dvisc	0.0002559	Paxs	369.65	Joback Method
dvisc	0.0001919	Paxs	403.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20680108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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