

Propane, 1,1-dimethoxy-

Other names:	Propionaldehyde, dimethyl acetal 1,1-Dimethoxypropane Propanal dimethyl acetal 3-Ethyl-2,4-dioxapentane DMP
Inchi:	InChI=1S/C5H12O2/c1-4-5(6-2)7-3/h5H,4H2,1-3H3
InchiKey:	UIOXNNAWANDJCZ-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CCC(OC)OC
Mol. weight [g/mol]:	104.15
CAS:	4744-10-9

Physical Properties

Property code	Value	Unit	Source
gf	-221.22	kJ/mol	Joback Method
hf	-416.25	kJ/mol	Joback Method
hfus	7.56	kJ/mol	Joback Method
hvap	31.16	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	1.015		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	658.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	650.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	880.00		NIST Webbook
tb	358.20	K	Joback Method
tc	527.59	K	Joback Method
tf	175.57	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.41	J/molxK	358.20	Joback Method
cpg	178.19	J/molxK	386.43	Joback Method
cpg	186.80	J/molxK	414.66	Joback Method
cpg	195.24	J/molxK	442.89	Joback Method
cpg	203.50	J/molxK	471.12	Joback Method
cpg	211.58	J/molxK	499.35	Joback Method
cpg	219.47	J/molxK	527.59	Joback Method
dvisc	0.0043341	Paxs	175.57	Joback Method
dvisc	0.0017713	Paxs	206.01	Joback Method
dvisc	0.0009115	Paxs	236.45	Joback Method
dvisc	0.0005458	Paxs	266.88	Joback Method
dvisc	0.0003630	Paxs	297.32	Joback Method
dvisc	0.0002604	Paxs	327.76	Joback Method
dvisc	0.0001977	Paxs	358.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4744109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/13-181-6/Propane-1-1-dimethoxy.pdf>

Generated by Cheméo on 2024-04-19 22:26:35.279930718 +0000 UTC m=+15854844.200508031.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.