

Propane, 1,1-diethoxy-2-methyl-

Other names:	Isobutyraldehyde, diethyl acetal Isobutanal diethyl acetal Isobutylaldehyde diethyl acetal 1,1-Diethoxy-2-methylpropane 1,1-Diethoxyisobutane
Inchi:	InChI=1S/C8H18O2/c1-5-9-8(7(3)4)10-6-2/h7-8H,5-6H2,1-4H3
InchiKey:	KZDFOVZPOBSHDH-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CCOC(OCC)C(C)C
Mol. weight [g/mol]:	146.23
CAS:	1741-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-198.40	kJ/mol	Joback Method
hf	-483.45	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	37.45	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	2.042		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	859.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	859.00		NIST Webbook
ripol	969.00		NIST Webbook
ripol	970.00		NIST Webbook
ripol	976.00		NIST Webbook
ripol	977.00		NIST Webbook
ripol	977.00		NIST Webbook

ripol	1000.00		NIST Webbook
ripol	969.00		NIST Webbook
ripol	962.00		NIST Webbook
tb	411.00 ± 4.00	K	NIST Webbook
tc	597.88	K	Joback Method
tf	194.38	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.44	J/mol×K	426.40	Joback Method
cpg	295.62	J/mol×K	454.98	Joback Method
cpg	308.43	J/mol×K	483.56	Joback Method
cpg	320.85	J/mol×K	512.14	Joback Method
cpg	332.88	J/mol×K	540.72	Joback Method
cpg	344.52	J/mol×K	569.30	Joback Method
cpg	355.77	J/mol×K	597.88	Joback Method
dvisc	0.0084710	Paxs	194.38	Joback Method
dvisc	0.0026002	Paxs	233.05	Joback Method
dvisc	0.0011171	Paxs	271.72	Joback Method
dvisc	0.0005924	Paxs	310.39	Joback Method
dvisc	0.0003615	Paxs	349.06	Joback Method
dvisc	0.0002435	Paxs	387.73	Joback Method
dvisc	0.0001762	Paxs	426.40	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=C1741419&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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