

Propane, 2,2-diethoxy-

Other names:	Acetone, diethyl acetal Acetone diethyl ketal 2,2-Diethoxypropane USAF do-44
Inchi:	InChI=1S/C7H16O2/c1-5-8-7(3,4)9-6-2/h5-6H2,1-4H3
InchiKey:	FGQLGYBGTRHODR-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCOC(C)(C)OCC
Mol. weight [g/mol]:	132.20
CAS:	126-84-1

Physical Properties

Property code	Value	Unit	Source
gf	-199.10	kJ/mol	Joback Method
hf	-506.70	kJ/mol	NIST Webbook
hfl	-538.50 ± 1.00	kJ/mol	NIST Webbook
hfus	8.85	kJ/mol	Joback Method
hvap	43.20 ± 0.40	kJ/mol	NIST Webbook
hvap	43.90	kJ/mol	NIST Webbook
hvap	31.80	kJ/mol	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.796		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	761.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	723.00		NIST Webbook
tb	386.00	K	NIST Webbook
tc	576.64	K	Joback Method
tf	207.90 ± 0.60	K	NIST Webbook
vc	0.453	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.99	J/molxK	401.17	Joback Method
cpg	256.60	J/molxK	430.42	Joback Method
cpg	268.75	J/molxK	459.66	Joback Method
cpg	280.46	J/molxK	488.91	Joback Method
cpg	291.74	J/molxK	518.15	Joback Method
cpg	302.58	J/molxK	547.40	Joback Method
cpg	312.99	J/molxK	576.64	Joback Method
dvisc	0.0049459	Paxs	215.53	Joback Method
dvisc	0.0021202	Paxs	246.47	Joback Method
dvisc	0.0010979	Paxs	277.41	Joback Method
dvisc	0.0006488	Paxs	308.35	Joback Method
dvisc	0.0004220	Paxs	339.29	Joback Method
dvisc	0.0002950	Paxs	370.23	Joback Method
dvisc	0.0002179	Paxs	401.17	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	318.20	K	8.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126841&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
hfl:	Liquid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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