

Propane, 1-(1-methylethoxy)-

Other names:	Ether, isopropyl propyl Isopropyl propyl ether Propyl isopropyl ether Propylisopropylether
Inchi:	InChI=1S/C6H14O/c1-4-5-7-6(2)3/h6H,4-5H2,1-3H3
InchiKey:	JIEJJGMNDWIGBJ-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCOC(C)C
Mol. weight [g/mol]:	102.17
CAS:	627-08-7

Physical Properties

Property code	Value	Unit	Source
gf	-107.80	kJ/mol	Joback Method
hf	-304.67	kJ/mol	Joback Method
hfus	8.96	kJ/mol	Joback Method
hvap	33.95	kJ/mol	NIST Webbook
log10ws	-1.34		Aqueous Solubility Prediction Method
log10ws	-1.34		Estimated Solubility Method
logp	1.821		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	609.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	593.00		NIST Webbook
ripol	708.00		NIST Webbook
ripol	708.00		NIST Webbook
tb	356.20	K	NIST Webbook
tb	356.20	K	NIST Webbook
tc	527.06	K	Joback Method
tf	164.61	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.69	J/mol×K	358.66	Joback Method
cpg	192.17	J/mol×K	386.73	Joback Method
cpg	202.35	J/mol×K	414.79	Joback Method
cpg	212.24	J/mol×K	442.86	Joback Method
cpg	221.82	J/mol×K	470.92	Joback Method
cpg	231.12	J/mol×K	498.99	Joback Method
cpg	240.11	J/mol×K	527.06	Joback Method
dvisc	0.0064749	Pa×s	164.61	Joback Method
dvisc	0.0023051	Pa×s	196.95	Joback Method
dvisc	0.0010982	Pa×s	229.29	Joback Method
dvisc	0.0006285	Pa×s	261.63	Joback Method
dvisc	0.0004067	Pa×s	293.98	Joback Method
dvisc	0.0002868	Pa×s	326.32	Joback Method
dvisc	0.0002155	Pa×s	358.66	Joback Method
hvapt	30.07	kJ/mol	356.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53446e+01
Coeff. B	-3.38994e+03
Coeff. C	-4.01600e+01
Temperature range (K), min.	265.30
Temperature range (K), max.	378.03

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C627087&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:
Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method:

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

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hvapt:	Enthalpy of vaporization at a given temperature
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
vc:	Critical Volume

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