

Propane, 1,1'-oxybis[2-methyl-

Other names:	1,1'-oxybis(2-methylpropane)
	1,1'-oxybis[2-methylpropane]
	1-isobutoxy-2-methylpropane
	2,6-dimethyl-4-oxaheptane
	Propane, 1,1'-oxybis*2-methyl-
	bis(2-methylpropyl) ether
	diisobutyl ether
Inchi:	InChI=1S/C8H18O/c1-7(2)5-9-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	SZNYWUQFZLLT-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)COCC(C)C
Mol. weight [g/mol]:	130.23
CAS:	628-55-7

Physical Properties

Property code	Value	Unit	Source
af	0.4476		Cheméo Relay (1.0)
hf	-346.11	kJ/mol	Cheméo Relay (1.0)
hfus	11.33	kJ/mol	Phase Equilibria and Thermodynamic Properties of Some Branched Alkyl Ethers
hvap	40.85	kJ/mol	NIST Webbook
hvap	41.20 ± 0.70	kJ/mol	NIST Webbook
ie	9.19	eV	Cheméo Relay (1.0)
log10ws	-2.86		Cheméo Relay (1.0)
logp	2.315		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	811.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	808.00		NIST Webbook
ripol	969.00		NIST Webbook
ripol	969.00		NIST Webbook
tb	395.70	K	NIST Webbook
tb	395.50 ± 0.50	K	NIST Webbook
tb	396.20	K	NIST Webbook

tc	577.66	K	Cheméo Relay (1.0)
tf	171.56	K	Cheméo Relay (1.0)
vc	0.483	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.23	J/mol×K	546.83	Joback Method
cpg	331.51	J/mol×K	575.40	Joback Method
cpg	308.52	J/mol×K	518.26	Joback Method
cpg	257.37	J/mol×K	403.98	Joback Method
cpg	270.82	J/mol×K	432.55	Joback Method
cpg	283.82	J/mol×K	461.12	Joback Method
cpg	296.39	J/mol×K	489.69	Joback Method
dvisc	0.0136903	Pa×s	172.15	Joback Method
dvisc	0.0035734	Pa×s	210.79	Joback Method
dvisc	0.0014141	Pa×s	249.43	Joback Method
dvisc	0.0007176	Pa×s	288.06	Joback Method
dvisc	0.0004275	Pa×s	326.70	Joback Method
dvisc	0.0002842	Pa×s	365.34	Joback Method
dvisc	0.0002043	Pa×s	403.98	Joback Method
hfust	11.33	kJ/mol	195.50	NIST Webbook
hvapt	38.90	kJ/mol	358.00	NIST Webbook
hvapt	33.95	kJ/mol	396.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54060e+01
Coeff. B	-3.71665e+03
Coeff. C	-5.11710e+01
Temperature range (K), min.	297.01
Temperature range (K), max.	419.36

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Cheméo Relay (1.0, beta):

Phase Equilibria and Thermodynamic
Properties of Some Branched Alkyl
Ethers
The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.doi.org/10.1021/je800998u>

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C628557&Units=SI>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Joback Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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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