

Propane, 1,1'-oxybis[3-chloro-

Other names:	Propane, 1,1'-oxybis*3-chloro-bis(3-chloropropyl) ether
Inchi:	InChI=1S/C6H12Cl2O/c7-3-1-5-9-6-2-4-8/h1-6H2
InchiKey:	SMANNJALMIGASX-UHFFFAOYSA-N
Formula:	C6H12Cl2O
SMILES:	CICCCOCCCCI
Mol. weight [g/mol]:	171.06
CAS:	629-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-129.22	kJ/mol	Joback Method
hf	-330.87	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	40.13	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	2.261		Crippen Method
mcvol	125.750	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
tb	433.96	K	Joback Method
tc	613.76	K	Joback Method
tf	239.45	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.34	J/mol×K	433.96	Joback Method
cpg	244.22	J/mol×K	463.93	Joback Method
cpg	253.74	J/mol×K	493.89	Joback Method
cpg	262.91	J/mol×K	523.86	Joback Method
cpg	271.73	J/mol×K	553.83	Joback Method
cpg	280.19	J/mol×K	583.80	Joback Method
cpg	288.31	J/mol×K	613.76	Joback Method

dvisc	0.0034436	Pa×s	239.45	Joback Method
dvisc	0.0017668	Pa×s	271.87	Joback Method
dvisc	0.0010450	Pa×s	304.29	Joback Method
dvisc	0.0006838	Pa×s	336.71	Joback Method
dvisc	0.0004821	Pa×s	369.12	Joback Method
dvisc	0.0003596	Pa×s	401.54	Joback Method
dvisc	0.0002803	Pa×s	433.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.20	K	99.30	NIST Webbook
tbrp	363.70	K	1.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629367&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1010.mol
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

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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