Cyclopropane, propyl-

Other names:	Propane, 1-cyclopropyl- Propylcyclopropane
Inchi:	InChI=1S/C6H12/c1-2-3-6-4-5-6/h6H,2-5H2,1H3
InchiKey:	MWVPQZRIWVPJCA-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	CCCC1CC1
Mol. weight [g/mol]:	84.16
CAS:	2415-72-7

Physical Properties

Property code	Value	Unit	Source
chl	-3770.00	kJ/mol	NIST Webbook
gf	60.39	kJ/mol	Joback Method
hf	-94.37	kJ/mol	Joback Method
hfus	9.43	kJ/mol	Joback Method
hvap	28.86	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.196		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	614.80		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	608.90		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	609.00		NIST Webbook
tb	342.30 ± 0.50	K	NIST Webbook
tb	342.65 ± 1.50	K	NIST Webbook
tb	341.65 ± 1.00	K	NIST Webbook
tc	521.85	K	Joback Method
tf	175.32	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.88	J/mol×K	343.42	Joback Method
cpg	196.23	J/mol×K	492.11	Joback Method
cpg	186.28	J/mol×K	462.37	Joback Method
cpg	175.79	J/mol×K	432.63	Joback Method
cpg	164.75	J/mol×K	402.90	Joback Method
cpg	153.12	J/mol×K	373.16	Joback Method
cpg	205.68	J/mol×K	521.85	Joback Method
dvisc	0.0002790	Pa×s	343.42	Joback Method
dvisc	0.0003062	Pa×s	315.40	Joback Method
dvisc	0.0003422	Pa×s	287.39	Joback Method
dvisc	0.0003917	Pa×s	259.37	Joback Method
dvisc	0.0004633	Pa×s	231.35	Joback Method
dvisc	0.0005740	Pa×s	203.34	Joback Method
dvisc	0.0007614	Pa×s	175.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52680e+01
Coeff. B	-3.25869e+03
Coeff. C	-3.63090e+01
Temperature range (K), min.	253.84
Temperature range (K), max.	363.60

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2415727&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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/mol455.mol

Legend

chl:	Standard liquid enthalpy of combustion
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume