1-Propylcyclopentene

Other names:	1-PROPYL-1-CYCLOPENTENE
	1-n-Propylcyclopentene
	Cyclopentene, 1-propyl-
Inchi:	InChI=1S/C8H14/c1-2-5-8-6-3-4-7-8/h6H,2-5,7H2,1H3
InchiKey:	FLWGCAJANMGQBB-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CCCC1=CCCC1
Mol. weight [g/mol]:	110.20
CAS:	3074-61-1

Physical Properties

Property code	Value	Unit	Source
gf	81.07	kJ/mol	Joback Method
hf	-81.32	kJ/mol	Joback Method
hfus	10.17	kJ/mol	Joback Method
hvap	34.92	kJ/mol	Joback Method
ie	8.48 ± 0.01	eV	NIST Webbook
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	839.20		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	836.50		NIST Webbook
rinpol	836.00		NIST Webbook

ripol	972.00		NIST Webbook
ripol	959.40		NIST Webbook
ripol	968.10		NIST Webbook
ripol	968.00		NIST Webbook
ripol	972.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	966.00		NIST Webbook
ripol	961.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	968.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	958.00		NIST Webbook
ripol	961.00		NIST Webbook
ripol	964.90		NIST Webbook
ripol	968.10		NIST Webbook
ripol	954.00		NIST Webbook
ripol	958.40		NIST Webbook
ripol	972.00		NIST Webbook
ripol	972.10		NIST Webbook
ripol	959.40		NIST Webbook
ripol	966.40		NIST Webbook
ripol	972.10		NIST Webbook
ripol	959.40		NIST Webbook
ripol	966.40		NIST Webbook
tb	405.20 ± 2.00	K	NIST Webbook
tb	405.00 ± 3.00	K	NIST Webbook
tb	452.00 ± 4.00	K	NIST Webbook
tc	603.30	K	Joback Method
tf	172.90 ± 0.50	K	NIST Webbook
tf	172.90 ± 2.00	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.93	J/mol×K	406.53	Joback Method
cpg	217.41	J/mol×K	439.32	Joback Method
cpg	231.16	J/mol×K	472.12	Joback Method
cpg	244.21	J/mol×K	504.91	Joback Method
cpg	256.57	J/mol×K	537.71	Joback Method
cpg	268.28	J/mol×K	570.50	Joback Method

cpg	279.37	J/mol×K	603.30	Joback Method
dvisc	0.0035547	Pa×s	208.34	Joback Method
dvisc	0.0017541	Pa×s	241.37	Joback Method
dvisc	0.0010260	Pa×s	274.40	Joback Method
dvisc	0.0006735	Pa×s	307.43	Joback Method
dvisc	0.0004797	Pa×s	340.47	Joback Method
dvisc	0.0003628	Pa×s	373.50	Joback Method
dvisc	0.0002871	Pa×s	406.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40000e+01
Coeff. B	-3.24721e+03
Coeff. C	-5.90780e+01
Temperature range (K), min.	295.89
Temperature range (K), max.	432.81

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3074611&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/mol635.mol

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
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