Cyclopentane, butyl-

Other names:	BUTYLCYCLOPENTANE
	n-Butylcyclopentane
Inchi:	InChI=1S/C9H18/c1-2-3-6-9-7-4-5-8-9/h9H,2-8H2,1H3
InchiKey:	ZAGHKONXGGSVDV-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CCCCC1CCCC1
Mol. weight [g/mol]:	126.24
CAS:	2040-95-1

Physical Properties

Property code	Value	Unit	Source
chl	-5899.90 ± 1.40	kJ/mol	NIST Webbook
gf	61.45	kJ/mol	Joback Method
hf	-168.30 ± 1.50	kJ/mol	NIST Webbook
hfl	-214.30 ± 1.50	kJ/mol	NIST Webbook
hfus	13.00	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
hvap	45.91	kJ/mol	NIST Webbook
ie	9.95 ± 0.03	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	929.40		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	938.30		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	929.80		NIST Webbook
rinpol	936.40		NIST Webbook
rinpol	937.20		NIST Webbook

rinpol	937.80		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	936.40		NIST Webbook
rinpol	937.10		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	935.85		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1001.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	971.00		NIST Webbook
ripol	979.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	993.80		NIST Webbook
ripol	988.90		NIST Webbook
ripol	1004.50		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	993.00		NIST Webbook
ripol	1000.50		NIST Webbook
ripol	996.70		NIST Webbook
ripol	989.00		NIST Webbook
ripol	1000.50		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	997.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	997.00		NIST Webbook
ripol	994.00		NIST Webbook
sg	453.80	J/mol×K	NIST Webbook
sl	343.84	J/mol×K	NIST Webbook
tb	429.85	K	KDB
tc	631.00	K	NIST Webbook

tf	164.95	K	KDB
tt	165.18 ± 0.01	K	NIST Webbook
tt	165.19 ± 0.60	K	NIST Webbook
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.49	J/mol×K	452.45	Joback Method
cpg	349.16	J/mol×K	611.72	Joback Method
cpg	335.53	J/mol×K	579.87	Joback Method
cpg	321.18	J/mol×K	548.02	Joback Method
cpg	306.07	J/mol×K	516.16	Joback Method
cpg	290.18	J/mol×K	484.31	Joback Method
cpg	255.97	J/mol×K	420.60	Joback Method
cpl	245.35	J/mol×K	298.15	NIST Webbook
dvisc	0.0011906	Pa×s	274.93	Joback Method
dvisc	0.0007556	Pa×s	311.35	Joback Method
dvisc	0.0005274	Pa×s	347.76	Joback Method
dvisc	0.0003941	Pa×s	384.18	Joback Method
dvisc	0.0003098	Pa×s	420.60	Joback Method
dvisc	0.0048336	Pa×s	202.09	Joback Method
dvisc	0.0021556	Pa×s	238.51	Joback Method
hfust	11.31	kJ/mol	165.18	NIST Webbook
hfust	11.31	kJ/mol	165.20	NIST Webbook
hfust	11.31	kJ/mol	165.20	NIST Webbook
hvapt	36.16	kJ/mol	429.80	NIST Webbook
hvapt	40.90 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	41.60 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	42.70 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	43.80 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	39.40	kJ/mol	422.50	NIST Webbook
sfust	68.49	J/mol×K	165.18	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42739e+01
Coeff. B	-3.58075e+03
Coeff. C	-5.90530e+01
Temperature range (K), min.	315.07
Temperature range (K), max.	458.58

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.37957e+01
Coeff. B	-8.62508e+03
Coeff. C	-1.16028e+01
Coeff. D	6.73064e-06
Temperature range (K), min.	314.15
Temperature range (K), max.	625.05

Sources

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/mol504.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040951&Units=SI

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=504

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume