Cyclopentene, 1-butyl-

Other names:	1-Butyl-1-cyclopentene
	1-Butylcyclopentene
Inchi:	InChI=1S/C9H16/c1-2-3-6-9-7-4-5-8-9/h7H,2-6,8H2,1H3
InchiKey:	MHIRRFYTMFZXHD-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CCCCC1=CCCC1
Mol. weight [g/mol]:	124.22
CAS:	2423-01-0

Physical Properties

Property code	Value	Unit	Source
gf	89.49	kJ/mol	Joback Method
hf	-101.96	kJ/mol	Joback Method
hfus	12.76	kJ/mol	Joback Method
hvap	37.15	kJ/mol	Joback Method
ie	8.45 ± 0.01	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	934.50		NIST Webbook
rinpol	937.70		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	938.00		NIST Webbook

ripol	1070.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1051.90		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1065.30		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1052.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1067.50		NIST Webbook
ripol	1071.30		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1056.20		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1070.50		NIST Webbook
ripol	1057.80		NIST Webbook
ripol	1065.30		NIST Webbook
ripol	1070.50		NIST Webbook
ripol	1057.80		NIST Webbook
ripol	1065.30		NIST Webbook
ripol	1051.90		NIST Webbook
tb	430.90 ± 1.50	K	NIST Webbook
tb	427.45 ± 0.70	K	NIST Webbook
tc	624.34	K	Joback Method
tf	219.61	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.91	J/mol×K	429.41	Joback Method
cpg	259.49	J/mol×K	461.90	Joback Method
cpg	274.30	J/mol×K	494.39	Joback Method

cpg	288.34	J/mol×K	526.88	Joback Method
cpg	301.67	J/mol×K	559.36	Joback Method
cpg	314.30	J/mol×K	591.85	Joback Method
cpg	326.26	J/mol×K	624.34	Joback Method
dvisc	0.0038690	Pa×s	219.61	Joback Method
dvisc	0.0018618	Pa×s	254.58	Joback Method
dvisc	0.0010691	Pa×s	289.54	Joback Method
dvisc	0.0006918	Pa×s	324.51	Joback Method
dvisc	0.0004873	Pa×s	359.48	Joback Method
dvisc	0.0003652	Pa×s	394.44	Joback Method
dvisc	0.0002869	Pa×s	429.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42977e+01
Coeff. B	-3.51999e+03
Coeff. C	-6.37900e+01
Temperature range (K), min.	315.04
Temperature range (K), max.	455.50

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol646.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2423010&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

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