Cyclopentane, 1-methyl-1-propyl-

Other names:	1-methyl-1-propylcyclopentane
	sec-Butylcyclopentane
Inchi:	InChI=1S/C9H18/c1-3-6-9(2)7-4-5-8-9/h3-8H2,1-2H3
InchiKey:	HICYLMKNNFKEMK-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CCCC1(C)CCCC1
Mol. weight [g/mol]:	126.24
CAS:	16631-63-3

Physical Properties

Property code	Value	Unit	Source
gf	55.96	kJ/mol	Joback Method
hf	-153.37	kJ/mol	Joback Method
hfus	6.70	kJ/mol	Joback Method
hvap	34.73	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	884.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	889.00		NIST Webbook
tb	420.84	K	Joback Method
tc	620.53	K	Joback Method
tf	225.99	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.85	J/mol×K	420.84	Joback Method
cpg	275.03	J/mol×K	454.12	Joback Method
cpg	292.03	J/mol×K	487.40	Joback Method
cpg	307.94	J/mol×K	520.68	Joback Method
cpg	322.85	J/mol×K	553.96	Joback Method
cpg	336.87	J/mol×K	587.24	Joback Method
cpg	350.08	J/mol×K	620.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37214e+01
Coeff. B	-3.28331e+03
Coeff. C	-6.18900e+01
Temperature range (K), min.	306.30
Temperature range (K), max.	452.30

Sources

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/mol508.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16631633&Units=SI

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

Legend

cpg: Ideal gas heat capacity

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