Cyclopentane, (1,1-dimethylethyl)-

Other names: tert-Butylcyclopentane
Inchi: InChI=1S/C9H18/c1-9(2,3)8-6-4-5-7-8/h8H,4-7H2,1-3H3
InchiKey: BFWVYBVSRYIDHI-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC(C)(C)C1CCCC1
Mol. weight [g/mol]: 126.24
CAS: 3875-52-3

Physical Properties

Property code	Value	Unit	Source
gf	64.29	kJ/mol	Joback Method
hf	-177.36	kJ/mol	Joback Method
hfus	5.59	kJ/mol	Joback Method
hvap	34.59	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	877.50		NIST Webbook
rinpol	881.30		NIST Webbook
tb	417.95 ± 0.20	K	NIST Webbook
tb	418.10 ± 1.00	K	NIST Webbook
tb	417.99 ± 0.20	K	NIST Webbook
tb	418.40 ± 1.00	K	NIST Webbook
tc	621.63	K	Joback Method
tf	204.51	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.50	J/mol×K	417.37	Joback Method
cpg	343.64	J/mol×K	587.58	Joback Method
cpg	328.46	J/mol×K	553.54	Joback Method

cpg	312.30	J/mol×K	519.50	Joback Method
cpg	295.12	J/mol×K	485.46	Joback Method
cpg	276.87	J/mol×K	451.41	Joback Method
cpg	357.89	J/mol×K	621.63	Joback Method
dvisc	0.0003296	Pa×s	417.37	Joback Method
dvisc	0.0004411	Pa×s	381.89	Joback Method
dvisc	0.0006266	Pa×s	346.42	Joback Method
dvisc	0.0009645	Pa×s	310.94	Joback Method
dvisc	0.0016588	Pa×s	275.46	Joback Method
dvisc	0.0033494	Pa×s	239.99	Joback Method
dvisc	0.0086296	Pa×s	204.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37426e+01
Coeff. B	-3.25078e+03
Coeff. C	-6.16710e+01
Temperature range (K), min.	303.28
Temperature range (K), max.	447.24

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/mol507.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3875523&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

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
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