Cyclopentanol, 1-methyl-

Other names: 1-Hydroxy-1-methylcyclopentane
1-Methyl-1-cyclopentanol
1-Methylcyclopentanol
Inchi: InChI=1S/C6H12O/c1-6(7)4-2-3-5-6/h7H,2-5H2,1H3
InchiKey: CAKWRXVKWGUISE-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC1(O)CCCC1
Mol. weight [g/mol]: 100.16
CAS: 1462-03-9

Physical Properties

Property code	Value	Unit	Source
chs	-3724.80 ± 1.10	kJ/mol	NIST Webbook
gf	-106.12	kJ/mol	Joback Method
hf	-285.00	kJ/mol	NIST Webbook
hf	-284.30 ± 1.40	kJ/mol	NIST Webbook
hfs	-352.00 ± 0.75	kJ/mol	NIST Webbook
hfs	-351.26	kJ/mol	NIST Webbook
hfus	3.02	kJ/mol	Joback Method
hsub	66.99 ± 0.15	kJ/mol	NIST Webbook
hsub	67.00	kJ/mol	NIST Webbook
hvap	44.73	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.311		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	4583.94	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	798.00		NIST Webbook
tb	408.70	K	NIST Webbook
tb	409.65 ± 2.00	K	NIST Webbook
tb	406.00 ± 3.00	K	NIST Webbook
tc	640.10	K	Joback Method

tf	308.65 ± 0.20	K	NIST Webbook
tf	309.00 ± 4.00	K	NIST Webbook
tf	297.80 ± 0.60	K	NIST Webbook
tf	309.00 ± 3.00	K	NIST Webbook
tf	306.00 ± 3.00	K	NIST Webbook
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.26	J/mol×K	444.38	Joback Method
cpg	202.53	J/mol×K	477.00	Joback Method
cpg	213.92	J/mol×K	509.62	Joback Method
cpg	224.53	J/mol×K	542.24	Joback Method
cpg	234.43	J/mol×K	574.86	Joback Method
cpg	243.72	J/mol×K	607.48	Joback Method
cpg	252.48	J/mol×K	640.10	Joback Method
hfust	8.41	kJ/mol	310.20	NIST Webbook
hfust	8.41	kJ/mol	310.20	NIST Webbook
hvapt	45.70	kJ/mol	380.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68739e+01
Coeff. B	-4.33609e+03
Coeff. C	-5.48940e+01
Temperature range (K), min.	316.32
Temperature range (K), max.	429.91

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1462039&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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