1-Propyl-1-cyclopentanol

Other names: 1-Propylcyclopentanol
Cyclopentanol, 1-propyl-
Inchi: InChI=1S/C8H16O/c1-2-5-8(9)6-3-4-7-8/h9H,2-7H2,1H3
InchiKey: GJEILRJIINEWJO-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCC1(O)CCCC1
Mol. weight [g/mol]: 128.21
CAS: 1604-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-89.28	kJ/mol	Joback Method
hf	-284.96	kJ/mol	Joback Method
hfus	8.20	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.092		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	446.70	K	NIST Webbook
tb	444.00 ± 3.00	K	NIST Webbook
tc	681.44	K	Joback Method
tf	275.54	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.14	J/mol×K	649.55	Joback Method
cpg	275.19	J/mol×K	490.14	Joback Method
cpg	289.15	J/mol×K	522.02	Joback Method
cpg	302.24	J/mol×K	553.91	Joback Method
cpg	314.54	J/mol×K	585.79	Joback Method
cpg	326.15	J/mol×K	617.67	Joback Method

cpg	347.60	J/mol×K	681.44	Joback Method
hvapt	64.20	kJ/mol	395.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.17961e+01
Coeff. B	-1.91677e+03
Coeff. C	-1.79658e+02
Temperature range (K), min.	346.21
Temperature range (K), max.	475.24

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=C1604020&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume