

1-Propylcyclopentanol

Other names:	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
hfus	8.20	kJ/mol	Joback Method
logp	2.092		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
tb	446.70	K	NIST Webbook
tb	444.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	337.14	J/mol×K	649.55	Joback Method
cpg	347.60	J/mol×K	681.44	Joback Method
hvapt	64.20	kJ/mol	395.50	NIST Webbook

Correlations

Information	Value
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Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1604020&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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