

Cyclopentanol, 1-ethyl-

Other names:	1-Ethyl-1-cyclopentanol 1-Ethylcyclopentanol
Inchi:	InChI=1S/C7H14O/c1-2-7(8)5-3-4-6-7/h8H,2-6H2,1H3
InchiKey:	LPCWIFPJLFCXRS-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCC1(O)CCCC1
Mol. weight [g/mol]:	114.19
CAS:	1462-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-97.70	kJ/mol	Joback Method
hf	-264.32	kJ/mol	Joback Method
hfus	5.61	kJ/mol	Joback Method
hvap	46.96	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.701		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	467.26	K	Joback Method
tc	660.80	K	Joback Method
tf	264.27	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.78	J/mol×K	467.26	Joback Method
cpg	244.94	J/mol×K	499.52	Joback Method
cpg	257.22	J/mol×K	531.77	Joback Method
cpg	268.72	J/mol×K	564.03	Joback Method
cpg	279.52	J/mol×K	596.29	Joback Method
cpg	289.70	J/mol×K	628.54	Joback Method
cpg	299.34	J/mol×K	660.80	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56660e+01
Coeff. B	-4.16482e+03
Coeff. C	-5.98980e+01
Temperature range (K), min.	330.72
Temperature range (K), max.	462.12

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1462960&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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

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