

1-Penten-3-ol

Other names:	1-Pentene-3-ol Ethyl vinyl carbinol Pent-1-en-3-ol ethylvinylcarbinol penten-3-ol «alpha»-Ethylallyl alcohol Â«alphaÂ»-Ethylallyl alcohol
Inchi:	InChI=1S/C5H10O/c1-3-5(6)4-2/h3,5-6H,1,4H2,2H3
InchiKey:	VHVMXWZXFBANQ-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	C=CC(O)CC
Mol. weight [g/mol]:	86.13
CAS:	616-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-60.20	kJ/mol	Joback Method
hf	-178.61	kJ/mol	Joback Method
hfus	7.99	kJ/mol	Joback Method
hvap	42.34	kJ/mol	Joback Method
ie	9.40 ± 0.05	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	0.943		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	672.00		NIST Webbook
rinpol	674.00		NIST Webbook
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ripol	1189.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1142.00		NIST Webbook
tb	388.20	K	NIST Webbook
tc	570.76	K	Joback Method
tf	190.17	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.13	J/molxK	514.58	Joback Method
cpg	198.29	J/molxK	570.76	Joback Method
cpg	191.86	J/molxK	542.67	Joback Method
cpg	155.14	J/molxK	402.22	Joback Method
cpg	163.12	J/molxK	430.31	Joback Method
cpg	170.77	J/molxK	458.40	Joback Method
cpg	178.10	J/molxK	486.49	Joback Method
dvisc	0.0002843	Paxs	402.22	Joback Method
dvisc	0.0010548	Paxs	331.54	Joback Method
dvisc	0.0005141	Paxs	366.88	Joback Method
dvisc	0.2702616	Paxs	190.17	Joback Method
dvisc	0.0351986	Paxs	225.51	Joback Method
dvisc	0.0079642	Paxs	260.85	Joback Method
dvisc	0.0025691	Paxs	296.19	Joback Method
hvapt	46.80 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	48.40 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	49.90 ± 0.10	kJ/mol	313.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58395e+01
Coeff. B	-3.80716e+03
Coeff. C	-4.89170e+01
Temperature range (K), min.	287.34
Temperature range (K), max.	410.54

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616251&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Activity Coefficients at Infinite Dilution of Volatile Compounds in Water: Effect of Temperature and Salt Concentration:	https://www.doi.org/10.1021/je2013878
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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