

1-Pentyn-3-ol

Other names:	Ethylethynylcarbinol Pent-1-yn-3-ol
Inchi:	InChI=1S/C5H8O/c1-3-5(6)4-2/h1,5-6H,4H2,2H3
InchiKey:	LBSKEFWQPNVWTP-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C#CC(O)CC
Mol. weight [g/mol]:	84.12
CAS:	4187-86-4

Physical Properties

Property code	Value	Unit	Source
gf	75.03	kJ/mol	Joback Method
hf	-12.14	kJ/mol	Joback Method
hfus	12.25	kJ/mol	Joback Method
hvap	42.87	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.390		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	397.00	K	NIST Webbook
tc	572.36	K	Joback Method
tf	238.90	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.04	J/mol×K	395.66	Joback Method
cpg	151.97	J/mol×K	425.11	Joback Method
cpg	158.59	J/mol×K	454.56	Joback Method
cpg	164.90	J/mol×K	484.01	Joback Method
cpg	170.92	J/mol×K	513.46	Joback Method
cpg	176.67	J/mol×K	542.91	Joback Method
cpg	182.15	J/mol×K	572.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64802e+01
Coeff. B	-4.09810e+03
Coeff. C	-5.15160e+01
Temperature range (K), min.	304.15
Temperature range (K), max.	418.15

Sources

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=C4187864&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

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
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

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