4-Pentyn-2-ol

Other names: 4-Pentyne-2-ol
pent-4-yn-2-ol
Inchi: InChI=1S/C5H8O/c1-3-4-5(2)6/h1,5-6H,4H2,2H3
InchiKey: JTHLRRZARWSHBE-UHFFFAOYSA-N
Formula: C5H8O
SMILES: C#CCC(C)O
Mol. weight [g/mol]: 84.12
CAS: 2117-11-5

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
ie	10.24	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	0.390		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	399.00	K	NIST Webbook
tb	399.70	K	NIST Webbook
tb	300.45 ± 0.50	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(Pvp) = A + B/(T + C)
Coeff. A	1.64795e+01
Coeff. B	-4.10284e+03
Coeff. C	-5.16780e+01
Temperature range (K), min.	305.15
Temperature range (K), max.	419.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2117115&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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

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