Ethylethynylcarbinol

Other names:	1-pentyn-3-ol
	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
hfus	12.25	kJ/mol	Joback Method
ie	10.27	eV	Cheméo Relay (1.0)
logp	0.390		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
tb	397.00	K	NIST Webbook

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	1.64802e+01
Coeff. B	-4.09810e+03
Coeff. C	-5.15160e+01
Temperature range (K), min.	304.15
Temperature range (K), max.	418.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4187864&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

Legend

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