1-Pentyn-3-ol, 3-ethyl-

Other names: 3-Aethyl-pentin-(1)-ol-(3)
3-Ethyl-1-pentyn-3-ol
3-Pentanol, 3-ethynyl-
3-ethylpent-1-yn-3-ol
Diethylethynylcarbinol
Inchi: InChI=1S/C7H12O/c1-4-7(8,5-2)6-3/h1,8H,5-6H2,2-3H3
InchiKey: PUNRPAWKFTXZIW-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C#CC(O)(CC)CC
Mol. weight [g/mol]: 112.17
CAS: 6285-06-9

Physical Properties

Property code	Value	Unit	Source
gf	97.15	kJ/mol	Joback Method
hf	-56.89	kJ/mol	Joback Method
hfus	13.53	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.171		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	409.50 ± 0.50	K	NIST Webbook
tb	411.15 ± 1.00	K	NIST Webbook
tc	620.20	K	Joback Method
tf	240.95 ± 3.00	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.13	J/mol×K	438.63	Joback Method
cpg	231.34	J/mol×K	468.89	Joback Method
cpg	240.97	J/mol×K	499.15	Joback Method

cpg	250.06	J/mol×K	529.41	Joback Method
cpg	258.64	J/mol×K	559.67	Joback Method
cpg	266.72	J/mol×K	589.93	Joback Method
cpg	274.35	J/mol×K	620.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64655e+01
Coeff. B	-4.19993e+03
Coeff. C	-5.49910e+01
Temperature range (K), min.	314.15
Temperature range (K), max.	431.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6285069&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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