1-Octen-3-yne

Other names: 1-Octene-3-yne
n-C4H9C«equiv»CCH=CH2
n-C4H9CÂ«equivÂ»CCH=CH2
Inchi: InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3H,1,4,6,8H2,2H3
InchiKey: UEKPKVCWUZMBML-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=CC#CCCCC
Mol. weight [g/mol]: 108.18
CAS: 17679-92-4

Physical Properties

Property code	Value	Unit	Source
gf	307.12	kJ/mol	Joback Method
hf	189.28	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	34.88	kJ/mol	Joback Method
ie	8.83 ± 0.01	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.366		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	407.00 ± 3.00	K	NIST Webbook
tc	579.51	K	Joback Method
tf	284.26	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.89	J/mol×K	388.12	Joback Method
cpg	205.28	J/mol×K	420.02	Joback Method
cpg	216.17	J/mol×K	451.92	Joback Method
cpg	226.59	J/mol×K	483.82	Joback Method
cpg	236.55	J/mol×K	515.72	Joback Method

cpg	246.07	J/mol×K	547.61	Joback Method
cpg	255.16	J/mol×K	579.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53674e+01
Coeff. B	-3.79081e+03
Coeff. C	-5.43380e+01
Temperature range (K), min.	305.72
Temperature range (K), max.	431.31

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17679924&Units=SI

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