2-Octyne

Other names: n-C5H11C«equiv»CCH3
n-C5H11CÂ«equivÂ»CCH3
oct-2-yne
Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3,5,7-8H2,1-2H3
InchiKey: QCQALVMFTWRCFI-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC#CCCCCC
Mol. weight [g/mol]: 110.20
CAS: 2809-67-8

Physical Properties

Property code	Value	Unit	Source
gf	219.28	kJ/mol	Joback Method
hf	63.80 ± 1.50	kJ/mol	NIST Webbook
hfus	19.60	kJ/mol	Joback Method
hvap	44.52	kJ/mol	NIST Webbook
hvap	44.50 ± 0.10	kJ/mol	NIST Webbook
ie	9.30 ± 0.01	eV	NIST Webbook
ie	9.31 ± 0.01	eV	NIST Webbook
ie	9.31 ± 0.02	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.590		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	842.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	863.00		NIST Webbook

rinpol	864.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	843.45		NIST Webbook
rinpol	843.46		NIST Webbook
rinpol	843.60		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	858.90		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	845.20		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	843.45		NIST Webbook
ripol	1041.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1054.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1040.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1059.00		NIST Webbook
ripol	1079.00		NIST Webbook
tb	410.35 ± 0.80	K	NIST Webbook
tb	411.15 ± 0.20	K	NIST Webbook

tb	410.88 ± 0.50	K	NIST Webbook
tb	407.15 ± 2.00	K	NIST Webbook
tb	410.70	K	NIST Webbook
tb	411.20	K	NIST Webbook
tb	411.00	K	NIST Webbook
tb	411.35 ± 0.50	K	NIST Webbook
tb	409.15 ± 1.50	K	NIST Webbook
tb	409.40 ± 1.50	K	NIST Webbook
tb	409.65 ± 1.50	K	NIST Webbook
tb	410.25 ± 0.50	K	NIST Webbook
tb	411.24 ± 0.60	K	NIST Webbook
tc	578.71	K	Joback Method
tf	211.55 ± 0.20	K	NIST Webbook
tf	211.15 ± 1.50	K	NIST Webbook
tf	211.44 ± 2.00	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.39	J/mol×K	391.44	Joback Method
cpg	220.42	J/mol×K	422.65	Joback Method
cpg	231.99	J/mol×K	453.86	Joback Method
cpg	243.10	J/mol×K	485.07	Joback Method
cpg	253.76	J/mol×K	516.28	Joback Method
cpg	264.00	J/mol×K	547.49	Joback Method
cpg	273.81	J/mol×K	578.71	Joback Method
hvapt	39.90	kJ/mol	390.00	NIST Webbook
hvapt	37.26	kJ/mol	410.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39125e+01
Coeff. B	-3.18531e+03
Coeff. C	-6.81600e+01

Temperature range (K), min.	301.95
Temperature range (K), max.	438.50

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.71593e+01
Coeff. B	-8.11149e+03
Coeff. C	-1.06258e+01
Coeff. D	6.73236e-06
Temperature range (K), min.	368.15
Temperature range (K), max.	412.00

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol429.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2809678&Units=SI

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=429

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

hvapt: Enthalpy of vaporization at a given temperature

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume