4-Octyne

Other names:	1,2-DIPROPYLACETYLENE
	DIPROPYLACETYLENE
	n-C3H7C«equiv»CC3H7
	n-C3H7CÂ«equivÂ»CC3H7
	oct-4-yne
Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-6H2,1-2H3
InchiKey:	GZTNBKQTTZSQNS-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CCCC#CCCC
Mol. weight [g/mol]:	110.20
CAS:	1942-45-6

Physical Properties

Property code	Value	Unit	Source
gf	219.28	kJ/mol	Joback Method
hf	60.10 ± 2.10	kJ/mol	NIST Webbook
hfus	19.60	kJ/mol	Joback Method
hvap	42.76	kJ/mol	NIST Webbook
hvap	42.70 ± 0.10	kJ/mol	NIST Webbook
ie	9.20 ± 0.02	eV	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.20 ± 0.01	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	811.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	809.90		NIST Webbook
rinpol	812.59		NIST Webbook
rinpol	812.51		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	813.60		NIST Webbook
rinpol	812.50		NIST Webbook

rinpol	813.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	810.60		NIST Webbook
rinpol	811.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	998.00		NIST Webbook
ripol	1011.60		NIST Webbook
ripol	999.00		NIST Webbook
tb	404.50 ± 0.50	K	NIST Webbook
tb	404.70	K	NIST Webbook
tb	404.00 ± 1.00	K	NIST Webbook
tb	404.70 ± 0.40	K	NIST Webbook
tb	404.64 ± 0.20	K	NIST Webbook
tb	404.64 ± 0.60	K	NIST Webbook
tb	404.72 ± 0.20	K	NIST Webbook
tb	404.80 ± 0.40	K	NIST Webbook
tb	404.67 ± 0.60	K	NIST Webbook
tb	406.00 ± 2.00	K	NIST Webbook
tb	406.00 ± 2.00	K	NIST Webbook
tb	404.56 ± 0.60	K	NIST Webbook
tb	404.70	K	NIST Webbook
tc	578.71	K	Joback Method
tf	286.02	K	Joback Method
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	39.60	kJ/mol	383.50	NIST Webbook
hvapt	36.00	kJ/mol	404.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40802e+01
Coeff. B	-3.23216e+03
Coeff. C	-6.31490e+01
Temperature range (K), min.	297.49
Temperature range (K), max.	431.75

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol431.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1942456&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
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015

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