1-Octyne

Other names: HEXYLACETYLENE
Octyne-1
oct-1-yne
Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h1H,4-8H2,2H3
InchiKey: UMIPWJGWASORKV-UHFFFAOYSA-N
Formula: C8H14
SMILES: C#CCCCCCC
Mol. weight [g/mol]: 110.20
CAS: 629-05-0

Physical Properties

Property code	Value	Unit	Source
gf	239.55	kJ/mol	Joback Method
hf	80.70 ± 3.60	kJ/mol	NIST Webbook
hfus	19.45	kJ/mol	Joback Method
hvap	42.34	kJ/mol	NIST Webbook
hvap	42.30 ± 0.10	kJ/mol	NIST Webbook
ie	9.95 ± 0.02	eV	NIST Webbook
log10ws	-3.66		Estimated Solubility Method
log10ws	-3.66		Aqueous Solubility Prediction Method
logp	2.590		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	787.50		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	783.60		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.50		NIST Webbook
rinpol	811.00		NIST Webbook

rinpol	812.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	788.10		NIST Webbook
rinpol	783.52		NIST Webbook
rinpol	785.80		NIST Webbook
rinpol	783.52		NIST Webbook
ripol	1047.10		NIST Webbook
ripol	1034.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1031.00		NIST Webbook
tb	372.56	K	Joback Method
tc	547.48	K	Joback Method
tf	200.38	K	Aqueous Solubility Prediction Method
tf	193.67 ± 0.10	K	NIST Webbook
tf	194.15 ± 1.50	K	NIST Webbook
tf	193.65 ± 0.30	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.74	J/mol×K	372.56	Joback Method
cpg	219.42	J/mol×K	401.71	Joback Method
cpg	230.61	J/mol×K	430.87	Joback Method
cpg	241.34	J/mol×K	460.02	Joback Method
cpg	251.62	J/mol×K	489.17	Joback Method
cpg	261.46	J/mol×K	518.33	Joback Method
cpg	270.87	J/mol×K	547.48	Joback Method
hvapt	35.83	kJ/mol	399.40	NIST Webbook
hvapt	38.50	kJ/mol	378.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.39482e+01
Coeff. B	-3.12653e+03
Coeff. C	-6.42400e+01
Temperature range (K), min.	293.11
Temperature range (K), max.	426.24

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.39993e+00
Coeff. B	-4.34412e+03
Coeff. C	3.22566e+00
Coeff. D	-8.94889e-06
Temperature range (K), min.	357.15
Temperature range (K), max.	400.15

Sources

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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