3-Octyne

Other names:	1-ETHYL-2-BUTYLACETYLENE
	BUTYLETHYLACETYLENE
	C4H9C«equiv»CC2H5
	C4H9CÂ«equivÂ»CC2H5
	Ethylbutylacetylene
	oct-3-yne
Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-5,7H2,1-2H3
InchiKey:	UDEISTCPVNLKRJ-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CCC#CCCCC
Mol. weight [g/mol]:	110.20
CAS:	15232-76-5

Physical Properties

Property code	Value	Unit	Source
gf	219.28	kJ/mol	Joback Method
hf	62.50 ± 1.80	kJ/mol	NIST Webbook
hfus	19.60	kJ/mol	Joback Method
hvap	43.95	kJ/mol	NIST Webbook
ie	9.22 ± 0.01	eV	NIST Webbook
ie	9.22 ± 0.01	eV	NIST Webbook
ie	9.22 ± 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	817.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	819.29		NIST Webbook
rinpol	819.37		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	820.70		NIST Webbook

rinpol	819.28		NIST Webbook
ripol	1012.00		NIST Webbook
ripol	1013.00		NIST Webbook
ripol	1012.00		NIST Webbook
ripol	1024.90		NIST Webbook
tb	391.44	K	Joback Method
tc	578.71	K	Joback Method
tf	169.25 ± 0.30	K	NIST Webbook
tf	162.71 ± 2.00	K	NIST Webbook
tf	168.15 ± 1.50	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.76	J/mol×K	516.28	Joback Method
cpg	264.00	J/mol×K	547.49	Joback Method
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	273.81	J/mol×K	578.71	Joback Method
hvapt	39.70	kJ/mol	384.50	NIST Webbook
hvapt	36.94	kJ/mol	406.30	NIST Webbook

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol430.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15232765&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=430

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
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