3-Octen-1-yne, (E)-

Other names: (E)-n-C4H9CH=CHC«equiv»CH
Inchi: InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h1,5,7H,4,6,8H2,2H3/b7-5+
InchiKey: FCNAWUZWKZOHKE-FNORWQNLSA-N
Formula: C8H12
SMILES: C#CC=CCCCC
Mol. weight [g/mol]: 108.18
CAS: 42104-42-7

Physical Properties

Property code	Value	Unit	Source
gf	319.77	kJ/mol	Joback Method
hf	200.67	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	33.22	kJ/mol	Joback Method
ie	8.87 ± 0.01	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.366		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	376.72	K	Joback Method
tc	561.02	K	Joback Method
tf	221.81	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.43	J/mol×K	376.72	Joback Method
cpg	204.91	J/mol×K	407.44	Joback Method
cpg	215.82	J/mol×K	438.15	Joback Method
cpg	226.17	J/mol×K	468.87	Joback Method
cpg	235.99	J/mol×K	499.59	Joback Method
cpg	245.30	J/mol×K	530.30	Joback Method
cpg	254.14	J/mol×K	561.02	Joback Method

Sources

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=C42104427&Units=SI
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume