

1-Octen-7-yne

Inchi:	InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h1,4H,2,5-8H2
InchiKey:	SNTQTQGMBSQRJZ-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C#CCCCC=C
Mol. weight [g/mol]:	108.18

Physical Properties

Property code	Value	Unit	Source
gf	327.39	kJ/mol	Joback Method
hf	208.88	kJ/mol	Joback Method
hfus	18.17	kJ/mol	Joback Method
hvap	32.59	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.366		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpola	765.70		NIST Webbook
tb	369.24	K	Joback Method
tc	547.90	K	Joback Method
tf	225.13	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.75	J/mol×K	369.24	Joback Method
cpg	204.84	J/mol×K	399.02	Joback Method
cpg	215.42	J/mol×K	428.79	Joback Method
cpg	225.51	J/mol×K	458.57	Joback Method
cpg	235.13	J/mol×K	488.34	Joback Method
cpg	244.30	J/mol×K	518.12	Joback Method
cpg	253.03	J/mol×K	547.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R144819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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