

1-HEXYN-3-ONE

Other names:	1-Hexyn-3-one 1-Hexyne-3-one Ethynyl propyl ketone Hex-1-yn-3-one
Inchi:	InChI=1S/C6H8O/c1-3-5-6(7)4-2/h2H,3,5H2,1H3
InchiKey:	KSJAIMUFADDAOP-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	C#CC(=O)CCC
Mol. weight [g/mol]:	96.13

Physical Properties

Property code	Value	Unit	Source
af	0.2948		Cheméo Relay (1.0)
gf	93.79	kJ/mol	Joback Method
hf	-44.59	kJ/mol	Cheméo Relay (1.0)
hfus	15.87	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Cheméo Relay (1.0)
ie	10.22 ± 0.04	eV	NIST Webbook
ie	9.94	eV	NIST Webbook
log10ws	-0.88		Cheméo Relay (1.0)
logp	0.989		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	374.51	K	Cheméo Relay (1.0)
tc	561.67	K	Cheméo Relay (1.0)
tf	242.81	K	Cheméo Relay (1.0)
vc	0.310	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.89	J/mol×K	380.67	Joback Method
cpg	162.24	J/mol×K	412.44	Joback Method
cpg	170.20	J/mol×K	444.21	Joback Method

cpg	177.78	J/mol×K	475.98	Joback Method
cpg	184.99	J/mol×K	507.75	Joback Method
cpg	191.86	J/mol×K	539.52	Joback Method
cpg	198.39	J/mol×K	571.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.70	K	13.30	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C689009&Units=SI>

Joback Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Legend

af:	Acentric Factor
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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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