3-OCTYNE-2-ONE

Other names:	3-Octyne-2-one
	Acetylbutylacetylene
	Butyl(acetyl)acetylene
	Oct-3-yn-2-one
Inchi:	InChI=1S/C8H12O/c1-3-4-5-6-7-8(2)9/h3-5H2,1-2H3
InchiKey:	VJKHTMGYHCBXHV-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCCCC#CC(C)=O
Mol. weight [g/mol]:	124.18

Physical Properties

Property code	Value	Unit	Source
af	0.3519		Cheméo Relay (1.0)
hf	-60.06	kJ/mol	Cheméo Relay (1.0)
hfus	21.20	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-1.66		Cheméo Relay (1.0)
logp	1.769		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	444.49	K	Cheméo Relay (1.0)
tc	617.23	K	Cheméo Relay (1.0)
tf	224.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.66	J/mol×K	445.31	Joback Method
cpg	238.08	J/mol×K	478.60	Joback Method
cpg	249.00	J/mol×K	511.89	Joback Method
cpg	259.44	J/mol×K	545.18	Joback Method
cpg	269.40	J/mol×K	578.47	Joback Method
cpg	278.91	J/mol×K	611.76	Joback Method

cpg	287.97	J/mol×K	645.05	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119580&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
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