

3-Butyne-2-one

Other names:	Methyl ethynyl ketone 1-Butyn-3-one Ketone, ethynyl methyl Ethynyl methyl ketone Acetylacetylene Acetylethyne But-3-yn-2-one 3-Butyne-2-one
Inchi:	InChI=1S/C4H4O/c1-3-4(2)5/h1H,2H3
InchiKey:	XRGPFNGLRSIPSA-UHFFFAOYSA-N
Formula:	C4H4O
SMILES:	C#CC(C)=O
Mol. weight [g/mol]:	68.07

Physical Properties

Property code	Value	Unit	Source
af	0.2109		Cheméo Relay (1.0)
gf	76.95	kJ/mol	Joback Method
hf	-4.50	kJ/mol	Cheméo Relay (1.0)
hfus	10.69	kJ/mol	Joback Method
hvap	30.86	kJ/mol	Cheméo Relay (1.0)
ie	10.25 ± 0.05	eV	NIST Webbook
ie	10.25	eV	NIST Webbook
ie	10.19	eV	NIST Webbook
ie	10.28	eV	NIST Webbook
ie	10.17	eV	NIST Webbook
logp	0.209		Crippen Method
mcvol	60.190	ml/mol	McGowan Method
pc	5168.28	kPa	Joback Method
tb	358.00	K	NIST Webbook
tc	521.42	K	Cheméo Relay (1.0)
tf	279.02	K	Cheméo Relay (1.0)
vc	0.211	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.64	J/mol×K	334.91	Joback Method
cpg	95.73	J/mol×K	366.91	Joback Method
cpg	100.56	J/mol×K	398.92	Joback Method
cpg	105.16	J/mol×K	430.92	Joback Method
cpg	109.53	J/mol×K	462.92	Joback Method
cpg	113.67	J/mol×K	494.93	Joback Method
cpg	117.61	J/mol×K	526.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	100.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1423605&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_{brp}:	Boiling point at reduced pressure
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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