2-Methyl-1-octen-3-yne

Other names: 2-Methyl-1-octene-3-yne
1-Octen-3-yne, 2-methyl-
2-Methyl-oct-1-en-3-yne
Inchi: InChI=1S/C9H14/c1-4-5-6-7-8-9(2)3/h2,4-6H2,1,3H3
InchiKey: FPKTZBDAOSTAHN-UHFFFAOYSA-N
Formula: C9H14
SMILES: C=C(C)C#CCCCC
Mol. weight [g/mol]: 122.21
CAS: 17603-76-8

Physical Properties

Property code	Value	Unit	Source
gf	306.99	kJ/mol	Joback Method
hf	158.85	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	37.19	kJ/mol	Joback Method
ie	8.57 ± 0.01	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	2.756		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	981.00		NIST Webbook
tb	410.88	K	Joback Method
tc	604.71	K	Joback Method
tf	281.57	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.84	J/mol×K	410.88	Joback Method
cpg	244.76	J/mol×K	443.19	Joback Method
cpg	257.10	J/mol×K	475.49	Joback Method
cpg	268.89	J/mol×K	507.80	Joback Method

cpg	280.15	J/mol×K	540.10	Joback Method
cpg	290.90	J/mol×K	572.41	Joback Method
cpg	301.14	J/mol×K	604.71	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.00 ± 1.00	K	4.80	NIST Webbook

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=C17603768&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume