3-Methoxyprop-1-yne

Other names: 1-Propyne, 3-methoxy-
3-Methoxy-1-propyne
3-Methoxyprop-1-yne
3-Methoxypropyne
Ether, methyl 2-propynyl
HC«equiv»CCH2OCH3
Methyl 2-propynyl ether
Propargyl methyl ether

Inchi: InChI=1S/C4H6O/c1-3-4-5-2/h1H,4H2,2H3

InchiKey: YACFFSVYSPMSGS-UHFFFAOYSA-N

Formula: C4H6O

SMILES: C#CCOC

Mol. weight [g/mol]: 70.09

Physical Properties

Property code	Value	Unit	Source
hf	57.50	kJ/mol	Cheméo Relay (1.0)
hfus	10.28	kJ/mol	Joback Method
hvap	29.96	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	NIST Webbook
logp	0.266		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
tb	334.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.08	J/mol×K	303.46	Joback Method
cpg	105.25	J/mol×K	332.70	Joback Method
cpg	110.28	J/mol×K	361.95	Joback Method
cpg	115.17	J/mol×K	391.19	Joback Method
cpg	119.94	J/mol×K	420.44	Joback Method
cpg	124.56	J/mol×K	449.68	Joback Method
cpg	129.05	J/mol×K	478.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627418&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

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature