2-METHYL-4-HEXYNE-3-ONE

Other names: 2-Methyl-4-hexyne-3-one
Inchi: InChI=1S/C7H10O/c1-4-5-7(8)6(2)3/h6H,1-3H3
InchiKey: XYKVPEZERYZDJY-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC#CC(=O)C(C)C
Mol. weight [g/mol]: 110.16

Physical Properties

Property code	Value	Unit	Source
hfus	15.08	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
logp	1.235		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
tb	399.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.19	J/mol×K	421.99	Joback Method
cpg	198.60	J/mol×K	456.47	Joback Method
cpg	208.55	J/mol×K	490.95	Joback Method
cpg	218.06	J/mol×K	525.43	Joback Method
cpg	227.13	J/mol×K	559.91	Joback Method
cpg	235.77	J/mol×K	594.39	Joback Method
cpg	244.00	J/mol×K	628.86	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52066338&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature