4-HEXYNE-3-ONE

Other names: 4-Hexyne-3-one
4-Hexyn-3-one
Inchi: InChI=1S/C6H8O/c1-3-5-6(7)4-2/h4H2,1-2H3
InchiKey: BIWUZTZFFUMZIG-UHFFFAOYSA-N
Formula: C6H8O
SMILES: CC#CC(=O)CC
Mol. weight [g/mol]: 96.13

Physical Properties

Property code	Value	Unit	Source
hfus	16.02	kJ/mol	Joback Method
ie	9.62	eV	NIST Webbook
logp	0.989		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
tb	401.97	K	Cheméo Relay (1.0)
tf	277.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.90	J/mol×K	399.55	Joback Method
cpg	160.46	J/mol×K	433.54	Joback Method
cpg	168.68	J/mol×K	467.54	Joback Method
cpg	176.55	J/mol×K	501.53	Joback Method
cpg	184.07	J/mol×K	535.52	Joback Method
cpg	191.27	J/mol×K	569.52	Joback Method
cpg	198.15	J/mol×K	603.51	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=C10575414&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
tf:	Normal melting (fusion) point