3-Pentyne-2-one

Other names: 3-Pentyn-2-one
3-Pentyne-2-one
Pent-3-yn-2-one
Inchi: InChI=1S/C5H6O/c1-3-4-5(2)6/h1-2H3
InchiKey: DZOOXMGZVWHNAS-UHFFFAOYSA-N
Formula: C5H6O
SMILES: CC#CC(C)=O
Mol. weight [g/mol]: 82.10

Physical Properties

Property code	Value	Unit	Source
hfus	13.43	kJ/mol	Joback Method
ie	9.76	eV	NIST Webbook
logp	0.599		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
tb	406.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.14	J/mol×K	376.67	Joback Method
cpg	125.04	J/mol×K	410.95	Joback Method
cpg	131.67	J/mol×K	445.23	Joback Method
cpg	138.04	J/mol×K	479.51	Joback Method
cpg	144.14	J/mol×K	513.79	Joback Method
cpg	149.99	J/mol×K	548.07	Joback Method
cpg	155.59	J/mol×K	582.35	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=C7299550&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