2-Heptyne-4-one

Other names: Hept-2-yn-4-one
Inchi: InChI=1S/C7H10O/c1-3-5-7(8)6-4-2/h3,5H2,1-2H3
InchiKey: NGDLDSJVXIMWCH-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC#CC(=O)CCC
Mol. weight [g/mol]: 110.15
CAS: 71932-98-4

Physical Properties

Property code	Value	Unit	Source
gf	81.94	kJ/mol	Joback Method
hf	-28.09	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	40.07	kJ/mol	Joback Method
ie	9.58	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	1.379		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	422.43	K	Joback Method
tc	624.38	K	Joback Method
tf	324.68	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.11	J/mol×K	422.43	Joback Method
cpg	198.18	J/mol×K	456.09	Joback Method
cpg	207.82	J/mol×K	489.75	Joback Method
cpg	217.05	J/mol×K	523.41	Joback Method
cpg	225.86	J/mol×K	557.07	Joback Method
cpg	234.28	J/mol×K	590.72	Joback Method
cpg	242.31	J/mol×K	624.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71932984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume