(E)-3-hexen-2-one

Other names: 3-hexen-2-one(E)
Inchi: InChI=1S/C6H10O/c1-3-4-5-6(2)7/h4-5H,3H2,1-2H3/b5-4+
InchiKey: LPCWMYHBLXLJJQ-SNAWJCMRSA-N
Formula: C6H10O
SMILES: CCC=CC(C)=O
Mol. weight [g/mol]: 98.14
CAS: 4376-23-2

Physical Properties

Property code	Value	Unit	Source
affp	865.60	kJ/mol	NIST Webbook
basg	833.80	kJ/mol	NIST Webbook
gf	-49.06	kJ/mol	Joback Method
hf	-162.53	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	35.65	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	843.00		NIST Webbook
rinpol	844.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1188.00		NIST Webbook
tb	394.71	K	Joback Method
tc	581.55	K	Joback Method
tf	202.23	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.73	J/mol×K	394.71	Joback Method
cpg	172.50	J/mol×K	425.85	Joback Method

cpg	181.81	J/mol×K	456.99	Joback Method
cpg	190.67	J/mol×K	488.13	Joback Method
cpg	199.09	J/mol×K	519.27	Joback Method
cpg	207.09	J/mol×K	550.41	Joback Method
cpg	214.70	J/mol×K	581.55	Joback Method
dvisc	0.0034897	Pa×s	202.23	Joback Method
dvisc	0.0016596	Pa×s	234.31	Joback Method
dvisc	0.0009440	Pa×s	266.39	Joback Method
dvisc	0.0006062	Pa×s	298.47	Joback Method
dvisc	0.0004242	Pa×s	330.55	Joback Method
dvisc	0.0003162	Pa×s	362.63	Joback Method
dvisc	0.0002472	Pa×s	394.71	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4376232&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

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