2-Pentanone, 3-methylene-

Other names: 3-Buten-2-one, 3-ethyl-
3-Methylene-2-pentanone
3-Ethyl-3-buten-2-one
Inchi: InChI=1S/C6H10O/c1-4-5(2)6(3)7/h2,4H2,1,3H3
InchiKey: UOTSYAILGSUTAC-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C=C(CC)C(C)=O
Mol. weight [g/mol]: 98.14
CAS: 4359-77-7

Physical Properties

Property code	Value	Unit	Source
gf	-49.99	kJ/mol	Joback Method
hf	-164.11	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	35.11	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
ripol	1137.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1128.00		NIST Webbook
tb	387.11	K	Joback Method
tc	572.11	K	Joback Method
tf	191.59	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.39	J/mol×K	387.11	Joback Method
cpg	172.98	J/mol×K	417.94	Joback Method
cpg	182.16	J/mol×K	448.78	Joback Method

cpg	190.92	J/mol×K	479.61	Joback Method
cpg	199.29	J/mol×K	510.45	Joback Method
cpg	207.28	J/mol×K	541.28	Joback Method
cpg	214.90	J/mol×K	572.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4359777&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume