5-Hexen-2-one, 5-methyl-3-methylene-

Inchi: InChI=1S/C8H12O/c1-6(2)5-7(3)8(4)9/h1,3,5H2,2,4H3
InchiKey: WEAGIKYKIOBREP-UHFFFAOYSA-N
Formula: C8H12O
SMILES: C=C(C)CC(=C)C(C)=O
Mol. weight [g/mol]: 124.18
CAS: 51756-18-4

Physical Properties

Property code	Value	Unit	Source
gf	46.14	kJ/mol	Joback Method
hf	-89.75	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	38.97	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	874.00		NIST Webbook
tb	429.43	K	Joback Method
tc	619.38	K	Joback Method
tf	198.41	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.60	J/mol×K	429.43	Joback Method
cpg	235.27	J/mol×K	461.09	Joback Method
cpg	246.36	J/mol×K	492.75	Joback Method
cpg	256.90	J/mol×K	524.40	Joback Method
cpg	266.91	J/mol×K	556.06	Joback Method

cpg	276.41	J/mol×K	587.72	Joback Method
cpg	285.42	J/mol×K	619.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51756184&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume