5-Hexenal, 4-methylene-

Other names: 4-Methylidenehex-5-enal
Inchi: InChI=1S/C7H10O/c1-3-7(2)5-4-6-8/h3,6H,1-2,4-5H2
InchiKey: GTQGBVLUEUNXCG-UHFFFAOYSA-N
Formula: C7H10O
SMILES: C=CC(=C)CCC=O
Mol. weight [g/mol]: 110.15
CAS: 17844-21-2

Physical Properties

Property code	Value	Unit	Source
gf	75.67	kJ/mol	Joback Method
hf	-32.32	kJ/mol	Joback Method
hfus	12.30	kJ/mol	Joback Method
hvap	36.64	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.708		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	896.80		NIST Webbook
rinpol	896.80		NIST Webbook
tb	401.46	K	Joback Method
tc	583.95	K	Joback Method
tf	193.17	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.15	J/mol×K	401.46	Joback Method
cpg	197.09	J/mol×K	431.87	Joback Method
cpg	206.56	J/mol×K	462.29	Joback Method
cpg	215.56	J/mol×K	492.70	Joback Method
cpg	224.12	J/mol×K	523.12	Joback Method
cpg	232.25	J/mol×K	553.53	Joback Method

cpg	239.97	J/mol×K	583.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17844212&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

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