2-Hexenal, 2-methyl-

Other names: (E)-2-Methyl-2-hexenal
Inchi: InChI=1S/C7H12O/c1-3-4-5-7(2)6-8/h5-6H,3-4H2,1-2H3/b7-5+
InchiKey: BRLKFSODKAIVGM-FNORWQNLSA-N
Formula: C7H12O
SMILES: CCCC=C(C)C=O
Mol. weight [g/mol]: 112.17
CAS: 28467-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-19.79	kJ/mol	Joback Method
hf	-165.96	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	37.93	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	884.00		NIST Webbook
tb	412.26	K	Joback Method
tc	596.19	K	Joback Method
tf	191.61	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.71	J/mol×K	412.26	Joback Method
cpg	212.62	J/mol×K	442.92	Joback Method
cpg	223.00	J/mol×K	473.57	Joback Method
cpg	232.88	J/mol×K	504.23	Joback Method
cpg	242.28	J/mol×K	534.88	Joback Method
cpg	251.22	J/mol×K	565.54	Joback Method
cpg	259.72	J/mol×K	596.19	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=C28467881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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