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
InchiKey: BRLKFSODKAIVGM-FNORWQNLSA-N
Formula: C7H12O
SMILES: CCC/C=C(\C)C=O
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
af	0.3459		Cheméo Relay (1.0)
gf	-19.79	kJ/mol	Joback Method
hf	-163.37	kJ/mol	Cheméo Relay (1.0)
hfus	15.07	kJ/mol	Joback Method
hvap	42.92	kJ/mol	Cheméo Relay (1.0)
ie	9.49	eV	Cheméo Relay (1.0)
log10ws	-1.85		Cheméo Relay (1.0)
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	884.00		NIST Webbook
rinpol	884.00		NIST Webbook
tb	425.30	K	Cheméo Relay (1.0)
tc	629.23	K	Cheméo Relay (1.0)
tf	187.46	K	Cheméo Relay (1.0)
vc	0.388	m3/kmol	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28467881&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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