(Z)-2-Hexenal

Other names: (Z)-Hex-2-enal
cis-2-hexenal
(Z)-hex-2-en-1-al
Inchi: InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3/b5-4-
InchiKey: MBDOYVRWFFCFHM-PLNGDYQASA-N
Formula: C6H10O
SMILES: CCCC=CC=O
Mol. weight [g/mol]: 98.14

Physical Properties

Property code	Value	Unit	Source
gf	-19.66	kJ/mol	Joback Method
hf	-135.53	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	855.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	850.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1189.00		NIST Webbook

ripol	1189.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1236.00		NIST Webbook
tb	389.50	K	Joback Method
tc	570.95	K	Joback Method
tf	194.30	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.69	J/mol×K	389.50	Joback Method
cpg	174.16	J/mol×K	419.74	Joback Method
cpg	183.18	J/mol×K	449.98	Joback Method
cpg	191.76	J/mol×K	480.23	Joback Method
cpg	199.93	J/mol×K	510.47	Joback Method
cpg	207.70	J/mol×K	540.71	Joback Method
cpg	215.09	J/mol×K	570.95	Joback Method

dvisc	0.0038680	Pa×s	194.30	Joback Method
dvisc	0.0017894	Pa×s	226.83	Joback Method
dvisc	0.0010044	Pa×s	259.37	Joback Method
dvisc	0.0006413	Pa×s	291.90	Joback Method
dvisc	0.0004480	Pa×s	324.43	Joback Method
dvisc	0.0003341	Pa×s	356.97	Joback Method
dvisc	0.0002617	Pa×s	389.50	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=R218138&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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