

Hexenal

Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3/b5-4+
InchiKey:	MBDOYVRWFFCFHM-SNAWJCMRSA-N
Formula:	C6H10O
SMILES:	CCCC=CC=O
Mol. weight [g/mol]:	98.14
CAS:	1335-39-3

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	776.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	788.00		NIST Webbook
ripol	1061.00		NIST Webbook
ripol	1061.00		NIST Webbook
tb	389.50	K	Joback Method
tc	570.95	K	Joback Method
tf	194.30	K	Joback Method
vc	0.368	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.69	J/molxK	389.50	Joback Method
cpg	174.16	J/molxK	419.74	Joback Method
cpg	183.18	J/molxK	449.98	Joback Method
cpg	191.76	J/molxK	480.23	Joback Method
cpg	199.93	J/molxK	510.47	Joback Method
cpg	207.70	J/molxK	540.71	Joback Method
cpg	215.09	J/molxK	570.95	Joback Method
dvisc	0.0038680	Paxs	194.30	Joback Method
dvisc	0.0017894	Paxs	226.83	Joback Method
dvisc	0.0010044	Paxs	259.37	Joback Method
dvisc	0.0006413	Paxs	291.90	Joback Method
dvisc	0.0004480	Paxs	324.43	Joback Method
dvisc	0.0003341	Paxs	356.97	Joback Method
dvisc	0.0002617	Paxs	389.50	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=C1335393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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