

# (E)-2-Pentenal

Inchi:	InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3/b4-3+
InchiKey:	DTCCTIQRPGSLPT-ONEGZZNKSA-N
Formula:	C5H8O
SMILES:	CCC=CC=O
Mol. weight [g/mol]:	84.12

## Physical Properties

Property code	Value	Unit	Source
gf	-28.08	kJ/mol	Joback Method
hf	-114.89	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	33.40	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	744.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	744.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1167.00		NIST Webbook
tb	366.62	K	Joback Method
tc	548.86	K	Joback Method
tf	183.03	K	Joback Method
vc	0.312	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.02	J/molxK	366.62	Joback Method
cpg	166.65	J/molxK	518.49	Joback Method
cpg	160.05	J/molxK	488.11	Joback Method

cpg	153.10	J/molxK	457.74	Joback Method
cpg	145.79	J/molxK	427.37	Joback Method
cpg	138.10	J/molxK	396.99	Joback Method
cpg	172.92	J/molxK	548.86	Joback Method
dvisc	0.0002502	Paxs	366.62	Joback Method
dvisc	0.0003168	Paxs	336.02	Joback Method
dvisc	0.0004205	Paxs	305.42	Joback Method
dvisc	0.0005946	Paxs	274.82	Joback Method
dvisc	0.0009169	Paxs	244.23	Joback Method
dvisc	0.0016007	Paxs	213.63	Joback Method
dvisc	0.0033669	Paxs	183.03	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R611344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R611344&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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