

# 2-Pentenal, (E)-

<b>Other names:</b>	(E)-2-Pentenal (E)-Pent-2-enal (E)-pent-2-en-1-al 2-(E)-Pentenal trans-2-Penten-1-al trans-2-Pentenal trans-Pent-2-enal
<b>Inchi:</b>	InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3/b4-3+
<b>InchiKey:</b>	DTCCTIQRPGSLPT-ONEGZZNKSA-N
<b>Formula:</b>	C5H8O
<b>SMILES:</b>	CCC=CC=O
<b>Mol. weight [g/mol]:</b>	84.12
<b>CAS:</b>	1576-87-0

## Physical Properties

Property code	Value	Unit	Source
affp	839.00	kJ/mol	NIST Webbook
basg	807.20	kJ/mol	NIST Webbook
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	724.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	746.00		NIST Webbook

rinpol	728.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	721.40	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	724.30	NIST Webbook
rinpol	724.30	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	744.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1134.00	NIST Webbook

ripol	1131.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1118.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1131.00	NIST Webbook
ripol	1134.00	NIST Webbook
ripol	1144.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1125.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1108.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1121.00	NIST Webbook
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ripol	1140.00	NIST Webbook
ripol	1127.00	NIST Webbook

ripol	1124.00		NIST Webbook
ripol	1125.00		NIST Webbook
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ripol	1111.00		NIST Webbook
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ripol	1147.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1124.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1117.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1139.00		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	138.10	J/molxK	396.99	Joback Method
cpg	145.79	J/molxK	427.37	Joback Method
cpg	153.10	J/molxK	457.74	Joback Method
cpg	160.05	J/molxK	488.11	Joback Method
cpg	166.65	J/molxK	518.49	Joback Method
cpg	172.92	J/molxK	548.86	Joback Method
dvisc	0.0033669	Paxs	183.03	Joback Method
dvisc	0.0016007	Paxs	213.63	Joback Method
dvisc	0.0009169	Paxs	244.23	Joback Method
dvisc	0.0005946	Paxs	274.82	Joback Method

dvisc	0.0004205	Paxs	305.42	Joback Method
dvisc	0.0003168	Paxs	336.02	Joback Method
dvisc	0.0002502	Paxs	366.62	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.70	K	21.30	NIST Webbook
tbrp	336.20	K	11.00	NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1576870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1576870&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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