2-Pentenal

Other names: Pent-2-enal
Inchi: InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3
InchiKey: DTCCTIQRPGSLPT-UHFFFAOYSA-N
Formula: C5H8O
SMILES: CCC=CC=O
Mol. weight [g/mol]: 84.12
CAS: 764-39-6

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
ie	9.70	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	676.77		NIST Webbook
rinpol	680.44		NIST Webbook
rinpol	682.23		NIST Webbook
rinpol	686.31		NIST Webbook
rinpol	700.44		NIST Webbook
rinpol	698.24		NIST Webbook
rinpol	699.75		NIST Webbook
rinpol	700.64		NIST Webbook
rinpol	701.70		NIST Webbook
rinpol	678.68		NIST Webbook
rinpol	704.71		NIST Webbook
rinpol	705.68		NIST Webbook
rinpol	707.08		NIST Webbook
rinpol	710.42		NIST Webbook
rinpol	713.43		NIST Webbook
rinpol	702.48		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	721.00		NIST Webbook

rinpol	721.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	717.73		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	675.36		NIST Webbook
rinpol	676.77		NIST Webbook
rinpol	682.23		NIST Webbook
rinpol	700.64		NIST Webbook
rinpol	707.08		NIST Webbook
rinpol	678.55		NIST Webbook
rinpol	675.72		NIST Webbook
rinpol	675.32		NIST Webbook
rinpol	674.91		NIST Webbook
rinpol	674.28		NIST Webbook
rinpol	675.36		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	677.72		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1078.94		NIST Webbook
ripol	1064.46		NIST Webbook
ripol	1043.68		NIST Webbook
ripol	1087.98		NIST Webbook
tb	397.00 ± 3.00	K	NIST Webbook
tc	548.86	K	Joback Method
tf	183.03	K	Joback Method
vc	0.312	m3/kmol	Joback Method

Temperature Dependent Properties

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

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49143e+01
Coeff. B	-3.55666e+03
Coeff. C	-5.15580e+01
Temperature range (K), min.	294.72
Temperature range (K), max.	421.93

Sources

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=C764396&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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