Pentanal

Other names:	1-Pentanal
	1-butanecarbaldehyde
	Amyl aldehyde
	Butyl formal
	N-PENTANAL
	NSC 35404
	Pentan-1-al
	Pentylaldehyde
	UN 2058
	VALERAL
	VALERIC ACID ALDEHYDE
	Valeraldehyde
	Valerianic aldehyde
	Valeric aldehyde
	Valeryl aldehyde
	butanecarbaldehyde
	n-C4H9CHO
	n-Valeraldehyde
	n-Valeric aldehyde
	pentanal (valeraldehyde)
	valderaldehyde
Inchi:	InChI=1S/C5H10O/c1-2-3-4-5-6/h5H,2-4H2,1H3
InchiKey:	HGBOYTHUEUWSSQ-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CCCCC=O
Mol. weight [g/mol]:	86.13
CAS:	110-62-3

Physical Properties

Property code	Value	Unit	Source
af	0.4000		KDB
affp	796.60	kJ/mol	NIST Webbook
basg	764.80	kJ/mol	NIST Webbook
dm	2.60	debye	KDB
gf	-108.40	kJ/mol	KDB
hf	-228.00	kJ/mol	KDB

hfus	10.99	kJ/mol	Joback Method
hvap	38.60	kJ/mol	NIST Webbook
hvap	38.10 ± 0.10	kJ/mol	NIST Webbook
hvap	38.30	kJ/mol	NIST Webbook
ie	9.89 ± 0.12	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.82 ± 0.05	eV	NIST Webbook
ie	9.82	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.74 ± 0.04	eV	NIST Webbook
ie	9.72 ± 0.06	eV	NIST Webbook
ie	9.65 ± 0.02	eV	NIST Webbook
ie	9.75 ± 0.01	eV	NIST Webbook
ie	9.77 ± 0.01	eV	NIST Webbook
log10ws	-0.85		Aqueous Solubility Prediction Method
log10ws	-0.85		Estimated Solubility Method
logp	1.375		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3970.00	kPa	KDB
pc	3970.00 ± 100.00	kPa	NIST Webbook
rhoc	274.76 ± 5.17	kg/m3	NIST Webbook
rinpol	664.10		NIST Webbook
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sg	379.90 ± 3.30	J/mol×K	NIST Webbook
sl	273.59	J/mol×K	NIST Webbook
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tb	375.15 ± 2.00	K	NIST Webbook
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tb	376.20	K	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
tb	376.00	K	KDB
tb	375.25 ± 2.00	K	NIST Webbook
tb	375.35 ± 1.50	K	NIST Webbook
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tf	191.59 ± 0.10	K	NIST Webbook
tf	182.15	K	NIST Webbook
tf	189.80 ± 1.00	K	NIST Webbook
tf	181.70 ± 3.00	K	NIST Webbook
vc	0.313	m3/kmol	KDB
zc	0.2640010		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.04	J/mol×K	420.08	Joback Method
cpg	144.57	J/mol×K	362.46	Joback Method
cpg	168.81	J/mol×K	448.89	Joback Method
cpg	176.29	J/mol×K	477.71	Joback Method
cpg	183.48	J/mol×K	506.52	Joback Method
cpg	190.38	J/mol×K	535.33	Joback Method
cpg	152.96	J/mol×K	391.27	Joback Method
cpl	174.39	J/mol×K	298.15	NIST Webbook
cpl	171.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0037054	Pa×s	188.11	Joback Method
dvisc	0.0018535	Pa×s	217.17	Joback Method
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dvisc	0.0003882	Pa×s	333.40	Joback Method
dvisc	0.0003071	Pa×s	362.46	Joback Method
hfust	15.00	kJ/mol	151.60	NIST Webbook
hvapt	33.64	kJ/mol	376.00	KDB
hvapt	37.30	kJ/mol	341.00	NIST Webbook
pvap	101.30	kPa	376.20	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	804.73	kg/m3	298.14	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	795.17	kg/m3	308.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	799.97	kg/m3	303.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	804.73	kg/m3	298.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction

rhol	790.33	kg/m3	313.14	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	809.45	kg/m3	293.14	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	814.15	kg/m3	288.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	810.00	kg/m3	293.00	KDB
rhol	785.46	kg/m3	318.14	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	780.55	kg/m3	323.14	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
srf	0.03	N/m	293.20	KDB

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction:	https://www.doi.org/10.1016/j.jct.2011.01.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1236.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sg:	Molar entropy at standard conditions

sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility