Butanal, 2-ethyl-

Other names:	(C2H5)2CHCHO
	2-Ethylbutanal
	2-Ethylbutyraldehyde
	2-Ethylbutyric aldehyde
	2-Ethylbutyric aledhyde
	3-Formylpentane
	Aldehyde 2-ethylbutyrique
	Butyraldehyde, 2-ethyl-
	Diethylacetaldehyde
	NSC 6757
	UN 1178
	«alpha»-Ethylbutanal
	«alpha»-Ethylbutyraldehyde
	Â«alphaÂ»-Ethylbutanal
	Â«alphaÂ»-Ethylbutyraldehyde
Inchi:	InChI=1S/C6H12O/c1-3-6(4-2)5-7/h5-6H,3-4H2,1-2H3
InchiKey:	UNNGUFMVYQJGTD-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCC(C=O)CC
Mol. weight [g/mol]:	100.16
CAS:	97-96-1

Physical Properties

Property code	Value	Unit	Source
ea	0.00 ± 0.00	eV	NIST Webbook
gf	-102.32	kJ/mol	Joback Method
hf	-258.03	kJ/mol	Joback Method
hfus	10.06	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
ie	9.54	eV	NIST Webbook
log10ws	-1.52		Estimated Solubility Method
log10ws	-1.52		Aqueous Solubility Prediction Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method

rinpol	748.85		NIST Webbook
rinpol	743.96		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	742.07		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	740.26		NIST Webbook
rinpol	746.25		NIST Webbook
rinpol	742.00		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	1032.70		NIST Webbook
ripol	1040.30		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1040.30		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	1025.30		NIST Webbook
ripol	1004.00		NIST Webbook
tb	384.90	K	Joback Method
tc	561.39	K	Joback Method
tf	184.00 ± 5.00	K	NIST Webbook
tf	184.15	K	NIST Webbook
tf	184.00 ± 4.00	K	NIST Webbook
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.50	J/mol×K	384.90	Joback Method
cpg	189.59	J/mol×K	414.32	Joback Method
cpg	199.28	J/mol×K	443.73	Joback Method
cpg	208.60	J/mol×K	473.15	Joback Method
cpg	217.54	J/mol×K	502.56	Joback Method
cpg	226.11	J/mol×K	531.98	Joback Method
cpg	234.32	J/mol×K	561.39	Joback Method
dvisc	0.0070161	Pa×s	184.38	Joback Method
dvisc	0.0027952	Pa×s	217.80	Joback Method

dvisc	0.0014226	Pa×s	251.22	Joback Method
dvisc	0.0008484	Pa×s	284.64	Joback Method
dvisc	0.0005641	Pa×s	318.06	Joback Method
dvisc	0.0004053	Pa×s	351.48	Joback Method
dvisc	0.0003084	Pa×s	384.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57429e+01
Coeff. B	-3.78669e+03
Coeff. C	-4.96120e+01
Temperature range (K), min.	294.62
Temperature range (K), max.	412.62

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97961&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

ea: Electron affinity

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