

Butanal, 2-methyl-

Other names:	(. +/-.)-2-Methylbutanal 2-Ethylpropanal 2-Formylbutane 2-Methyl-1-butanal 2-Methylbutanal 2-Methylbutyraldehyde 2-Methylbutyric aldehyde Acetaldehyde, ethylmethyl- Butyraldehyde, 2-methyl- Methylethylacetaldehyde NSC 77077 sec-C4H9CHO «alpha»-Methylbutanal «alpha»-Methylbutyraldehyde «alpha»-Methylbutyric aldehyde Â«alphaÂ»-Methylbutanal Â«alphaÂ»-Methylbutyraldehyde Â«alphaÂ»-Methylbutyric aldehyde
Inchi:	InChI=1S/C5H10O/c1-3-5(2)4-6/h4-5H,3H2,1-2H3
InchiKey:	BYGQBDHUGHBGMD-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CCC(C)C=O
Mol. weight [g/mol]:	86.13
CAS:	96-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-110.74	kJ/mol	Joback Method
hf	-237.39	kJ/mol	Joback Method
hfus	7.47	kJ/mol	Joback Method
hvap	33.06	kJ/mol	Joback Method
ie	9.59 ± 0.01	eV	NIST Webbook
log10ws	-0.95		Crippen Method
logp	1.231		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	664.00		NIST Webbook

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ripol	913.00		NIST Webbook
tb	362.02	K	Joback Method
tc	539.07	K	Joback Method
tf	167.70 ± 0.70	K	NIST Webbook
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.45	J/mol×K	362.02	Joback Method
cpg	153.14	J/mol×K	391.53	Joback Method
cpg	161.50	J/mol×K	421.04	Joback Method
cpg	169.54	J/mol×K	450.54	Joback Method
cpg	177.25	J/mol×K	480.05	Joback Method
cpg	184.66	J/mol×K	509.56	Joback Method
cpg	191.76	J/mol×K	539.07	Joback Method
dvisc	0.0063146	Pa×s	173.11	Joback Method
dvisc	0.0025690	Pa×s	204.59	Joback Method
dvisc	0.0013285	Pa×s	236.08	Joback Method

dvisc	0.0008023	Pa×s	267.56	Joback Method
dvisc	0.0005388	Pa×s	299.05	Joback Method
dvisc	0.0003904	Pa×s	330.53	Joback Method
dvisc	0.0002992	Pa×s	362.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46588e+01
Coeff. B	-3.08091e+03
Coeff. C	-5.81500e+01
Temperature range (K), min.	272.53
Temperature range (K), max.	387.75

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=C96173&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
Limiting Separation Factors and Limiting Activity Coefficients for Hexanal, 2-Methylbutanal, 3-Methylbutanal, and Dimethylsulfide in Water at (98.1 to 99.0) deg C:	https://www.doi.org/10.1021/je060324o

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

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