

Butanal, 3-methyl-

Other names:	1-Butanal, 3-methyl- 2-Methylbutanal-4 3-Methyl-1-butanal 3-Methylbutan-1-al 3-Methylbutanal 3-Methylbutyraldehyde Butyraldehyde, 3-methyl- Isoamylaldehyde Isopentaldehyde Isopentanal Isovaleral Isovaleraldehyde Isovaleric aldehyde Isovalerylaldehyde NSC 404119 iso-C4H9CHO «beta»-Methylbutanal Â«betaÂ»-Methylbutanal
Inchi:	InChI=1S/C5H10O/c1-5(2)3-4-6/h4-5H,3H2,1-2H3
InchiKey:	YGHRJJRRZDOVPD-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC(C)CC=O
Mol. weight [g/mol]:	86.13
CAS:	590-86-3

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	9.71 ± 0.05	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.68 ± 0.02	eV	NIST Webbook
ie	9.70 ± 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	628.00		NIST Webbook
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tb	362.02	K	Joback Method
tc	539.07	K	Joback Method
tf	167.70 ± 1.00	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	184.66	J/mol×K	509.56	Joback Method
cpg	177.25	J/mol×K	480.05	Joback Method
cpg	169.54	J/mol×K	450.54	Joback Method
cpg	161.50	J/mol×K	421.04	Joback Method
cpg	153.14	J/mol×K	391.53	Joback Method

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dvisc	0.0025690	Pa×s	204.59	Joback Method
dvisc	0.0063146	Pa×s	173.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45335e+01
Coeff. B	-3.04644e+03
Coeff. C	-5.81500e+01
Temperature range (K), min.	272.00
Temperature range (K), max.	388.49

Sources

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 Aqueous Solutions at Infinite Dilution of Volatile Compounds in Water: Effect of Temperature and Salt Concentration:	https://www.doi.org/10.1021/je060324o
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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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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