Butanal, 3,3-dimethyl-

Other names:	3,3-dimethylbutanal
	3,3-dimethylbutyraldehyde
Inchi:	InChI=1S/C6H12O/c1-6(2,3)4-5-7/h5H,4H2,1-3H3
InchiKey:	LTNUSYNQZJZUSY-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC(C)(C)CC=O
Mol. weight [g/mol]:	100.16
CAS:	2987-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-97.04	kJ/mol	Joback Method
hf	-261.50	kJ/mol	Joback Method
hfus	6.17	kJ/mol	Joback Method
hvap	34.37	kJ/mol	Joback Method
ie	9.61 ± 0.01	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	697.00		NIST Webbook
rinpol	694.01		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	691.42		NIST Webbook
rinpol	689.09		NIST Webbook
rinpol	687.24		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	697.02		NIST Webbook
ripol	969.00		NIST Webbook
ripol	981.40		NIST Webbook
ripol	974.80		NIST Webbook
ripol	968.60		NIST Webbook
ripol	988.30		NIST Webbook

tb	380.15 ± 3.00	K	NIST Webbook
tb	376.00 ± 4.00	K	NIST Webbook
tb	375.90 ± 2.00	K	NIST Webbook
tc	566.17	K	Joback Method
tf	201.80	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.97	J/mol×K	382.11	Joback Method
cpg	231.30	J/mol×K	535.49	Joback Method
cpg	222.30	J/mol×K	504.82	Joback Method
cpg	212.79	J/mol×K	474.14	Joback Method
cpg	202.74	J/mol×K	443.46	Joback Method
cpg	192.15	J/mol×K	412.79	Joback Method
cpg	239.82	J/mol×K	566.17	Joback Method
dvisc	0.0003588	Pa×s	382.11	Joback Method
dvisc	0.0004807	Pa×s	352.06	Joback Method
dvisc	0.0006800	Pa×s	322.01	Joback Method
dvisc	0.0010332	Pa×s	291.96	Joback Method
dvisc	0.0017279	Pa×s	261.90	Joback Method
dvisc	0.0033020	Pa×s	231.85	Joback Method
dvisc	0.0076524	Pa×s	201.80	Joback Method

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=C2987168&Units=SI
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
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