

Butanal, 2,2-dimethyl-

Inchi:	InChI=1S/C6H12O/c1-4-6(2,3)5-7/h5H,4H2,1-3H3
InchiKey:	QYPLKDUOPJZROX-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCC(C)(C)C=O
Mol. weight [g/mol]:	100.16
CAS:	2094-75-9

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
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	377.15 ± 2.00	K	NIST Webbook
tb	378.40 ± 1.50	K	NIST Webbook
tb	376.15 ± 3.00	K	NIST Webbook
tc	566.17	K	Joback Method
tf	201.80	K	Joback Method
vc	0.378	m ³ /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	Paxs	382.11	Joback Method
dvisc	0.0004807	Paxs	352.06	Joback Method
dvisc	0.0006800	Paxs	322.01	Joback Method
dvisc	0.0010332	Paxs	291.96	Joback Method
dvisc	0.0017279	Paxs	261.90	Joback Method
dvisc	0.0033020	Paxs	231.85	Joback Method
dvisc	0.0076524	Paxs	201.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2094759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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