3,3-Dimethylbutanal

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
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	689.00		NIST Webbook
tb	382.11	K	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49724e+01
Coeff. B	-3.55037e+03
Coeff. C	-4.78880e+01
Temperature range (K), min.	289.66
Temperature range (K), max.	415.39

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R602003&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

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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume