Butanoic acid, 3,3-dimethyl-

Other names:	(CH3)3CCH2COOH
	3,3-Dimethyl-n-butyric acid
	3,3-Dimethylbutanoic acid
	3,3-Dimethylbutyric acid
	Butyric acid, 3,3-dimethyl-
	t-Butylacetic acid
	tert-Butylacetic acid
Inchi:	InChI=1S/C6H12O2/c1-6(2,3)4-5(7)8/h4H2,1-3H3,(H,7,8)
InchiKey:	MLMQPDHYNJCQAO-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC(C)(C)CC(=O)O
Mol. weight [g/mol]:	116.16
CAS:	1070-83-3

Physical Properties

Property code	Value	Unit	Source
gf	-263.26	kJ/mol	Joback Method
hf	-440.73	kJ/mol	Joback Method
hfus	9.57	kJ/mol	Joback Method
hvap	64.00 ± 0.90	kJ/mol	NIST Webbook
log10ws	-1.19		Crippen Method
logp	1.507		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	463.20	K	NIST Webbook
tb	460.70	K	NIST Webbook
tc	661.11	K	Joback Method
tf	280.00 ± 2.00	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.86	J/mol×K	479.50	Joback Method

cpg	236.61	J/mol×K	509.77	Joback Method
cpg	245.85	J/mol×K	540.04	Joback Method
cpg	254.59	J/mol×K	570.30	Joback Method
cpg	262.86	J/mol×K	600.57	Joback Method
cpg	270.68	J/mol×K	630.84	Joback Method
cpg	278.06	J/mol×K	661.11	Joback Method
dvisc	0.0298236	Pa×s	270.55	Joback Method
dvisc	0.0081361	Pa×s	305.38	Joback Method
dvisc	0.0028958	Pa×s	340.20	Joback Method
dvisc	0.0012487	Pa×s	375.02	Joback Method
dvisc	0.0006212	Pa×s	409.85	Joback Method
dvisc	0.0003447	Pa×s	444.67	Joback Method
dvisc	0.0002084	Pa×s	479.50	Joback Method
hvapt	63.60 ± 0.90	kJ/mol	304.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57473e+01
Coeff. B	-4.34913e+03
Coeff. C	-6.99060e+01
Temperature range (K), min.	351.23
Temperature range (K), max.	486.66

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1070833&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume