Butanoic acid, 2-oxo-

Other names:	Butyric acid, 2-oxo-
	2-Ketobutyric acid
	2-Ketobutanoic acid
	«alpha»-Ketobutyric acid
	2-Oxobutyric acid
	«alpha»-Keto-n-butyric acid
	«alpha»-Ketobutric acid
	«alpha»-Oxo-n-butyric acid
	Formic acid, propionyl-
	Pyruvic acid, methyl-
	2-Oxobutanoic acid
	3-Methylpyruvic acid
	NSC 60533
	2-Oxo-n-butyric acid
	«alpha»-Oxobutyric acid
	alpha-Oxobutanoic acid
Inchi:	InChI=1S/C4H6O3/c1-2-3(5)4(6)7/h2H2,1H3,(H,6,7)
InchiKey:	TYEYBOSBBBHJIV-UHFFFAOYSA-N
Formula:	C4H6O3
SMILES:	CCC(=O)C(=O)O
Mol. weight [g/mol]:	102.09
CAS:	600-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-411.86	kJ/mol	Joback Method
hf	-503.28	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	54.67	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	0.050		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
rinpol	847.70		NIST Webbook
rinpol	847.70		NIST Webbook
tb	490.84	K	Joback Method
tc	675.00	K	Joback Method

tf	295.52	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.18	J/mol×K	490.84	Joback Method
cpg	161.14	J/mol×K	521.53	Joback Method
cpg	166.84	J/mol×K	552.23	Joback Method
cpg	172.27	J/mol×K	582.92	Joback Method
cpg	177.44	J/mol×K	613.62	Joback Method
cpg	182.36	J/mol×K	644.31	Joback Method
cpg	187.03	J/mol×K	675.00	Joback Method
dvisc	0.0117823	Pa×s	295.52	Joback Method
dvisc	0.0044513	Pa×s	328.07	Joback Method
dvisc	0.0020048	Pa×s	360.63	Joback Method
dvisc	0.0010304	Pa×s	393.18	Joback Method
dvisc	0.0005863	Pa×s	425.73	Joback Method
dvisc	0.0003615	Pa×s	458.29	Joback Method
dvisc	0.0002376	Pa×s	490.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	2.70	NIST Webbook

Sources

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=C600180&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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