

Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester

Other names:	Acetoacetic acid, tert-butyl ester tert-Butyl Acetoacetate tert-Butyl 3-Oxobutyrate t-Butyl acetoacetate ter'-Butylacetoacetate 3,3-dimethylbutyryl chloride
Inchi:	InChI=1S/C8H14O3/c1-6(9)5-7(10)11-8(2,3)4/h5H2,1-4H3
InchiKey:	JKUYRAMKJLMYLO-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CC(=O)CC(=O)OC(C)(C)C
Mol. weight [g/mol]:	158.19
CAS:	1694-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-343.52	kJ/mol	Joback Method
hf	-574.58	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.307		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	457.00	K	NIST Webbook
tc	705.37	K	Joback Method
tf	304.43	K	Joback Method
vc	0.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.98	J/mol×K	509.37	Joback Method
cpg	314.46	J/mol×K	542.04	Joback Method
cpg	326.31	J/mol×K	574.70	Joback Method

cpg	337.53	J/molxK	607.37	Joback Method
cpg	348.15	J/molxK	640.04	Joback Method
cpg	358.18	J/molxK	672.71	Joback Method
cpg	367.64	J/molxK	705.37	Joback Method
dvisc	0.0033814	Paxs	304.43	Joback Method
dvisc	0.0017905	Paxs	338.59	Joback Method
dvisc	0.0010652	Paxs	372.74	Joback Method
dvisc	0.0006915	Paxs	406.90	Joback Method
dvisc	0.0004799	Paxs	441.06	Joback Method
dvisc	0.0003511	Paxs	475.21	Joback Method
dvisc	0.0002678	Paxs	509.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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