Butanoic acid, 3-oxo-, butyl ester

Other names:	Acetoacetic acid, butyl ester
	Butyl acetoacetate
	Butylester kyseliny acetoctove
Inchi:	InChI=1S/C8H14O3/c1-3-4-5-11-8(10)6-7(2)9/h3-6H2,1-2H3
InchiKey:	REIYHFWZISXFKU-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CCCCOC(=O)CC(C)=O
Mol. weight [g/mol]:	158.19
CAS:	591-60-6

Physical Properties

Property code	Value	Unit	Source
gf	-346.36	kJ/mol	Joback Method
hf	-565.83	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.309		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
ripol	1798.00		NIST Webbook
tb	512.60	K	Joback Method
tc	697.35	K	Joback Method
tf	302.01	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.67	J/mol×K	512.60	Joback Method
cpg	351.97	J/mol×K	666.56	Joback Method
cpg	342.23	J/mol×K	635.77	Joback Method

cpg	332.03	J/mol×K	604.98	Joback Method
cpg	321.37	J/mol×K	574.18	Joback Method
cpg	310.25	J/mol×K	543.39	Joback Method
cpg	361.25	J/mol×K	697.35	Joback Method
dvisc	0.0002790	Pa×s	512.60	Joback Method
dvisc	0.0003549	Pa×s	477.50	Joback Method
dvisc	0.0004690	Pa×s	442.40	Joback Method
dvisc	0.0006504	Pa×s	407.31	Joback Method
dvisc	0.0009592	Pa×s	372.21	Joback Method
dvisc	0.0015339	Pa×s	337.11	Joback Method
dvisc	0.0027356	Pa×s	302.01	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591606&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume