Butanoic acid, 3-oxo-, 2-methylpropyl ester

Other names:	Acetoacetic acid, isobutyl ester
	Isobutyl acetoacetate
	2-Methyl-1-propyl acetoacetate
	Isobutyl 3-ketobutanoate
	Isobutyl 3-ketobutyrate
Inchi:	InChI=1S/C8H14O3/c1-6(2)5-11-8(10)4-7(3)9/h6H,4-5H2,1-3H3
InchiKey:	ZYXNLVMBIHVDRH-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CC(=O)CC(=O)OCC(C)C
Mol. weight [g/mol]:	158.19
CAS:	7779-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-348.80	kJ/mol	Joback Method
hf	-571.11	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.165		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	477.00	K	NIST Webbook
tc	700.78	K	Joback Method
tf	287.01	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.94	J/mol×K	512.16	Joback Method
cpg	310.84	J/mol×K	543.60	Joback Method

cpg	322.24	J/mol×K	575.03	Joback Method
cpg	333.16	J/mol×K	606.47	Joback Method
cpg	343.58	J/mol×K	637.91	Joback Method
cpg	353.52	J/mol×K	669.35	Joback Method
cpg	362.98	J/mol×K	700.78	Joback Method
dvisc	0.0036492	Pa×s	287.01	Joback Method
dvisc	0.0018279	Pa×s	324.53	Joback Method
dvisc	0.0010567	Pa×s	362.06	Joback Method
dvisc	0.0006771	Pa×s	399.58	Joback Method
dvisc	0.0004683	Pa×s	437.11	Joback Method
dvisc	0.0003434	Pa×s	474.63	Joback Method
dvisc	0.0002635	Pa×s	512.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	2.90	NIST Webbook

Sources

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=C7779751&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	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