

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

Other names:	Acetoacetic acid, sec-butyl ester sec-Butyl Acetoacetate
Inchi:	InChI=1S/C8H14O3/c1-4-7(3)11-8(10)5-6(2)9/h7H,4-5H2,1-3H3
InchiKey:	QSTNBMLCULGCQE-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CCC(C)OC(=O)CC(C)=O
Mol. weight [g/mol]:	158.19
CAS:	13562-76-0

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	-1.43		Crippen Method
logp	1.307		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	467.00	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/molxK	512.16	Joback Method
cpg	310.84	J/molxK	543.60	Joback Method
cpg	322.24	J/molxK	575.03	Joback Method
cpg	333.16	J/molxK	606.47	Joback Method
cpg	343.58	J/molxK	637.91	Joback Method
cpg	353.52	J/molxK	669.35	Joback Method
cpg	362.98	J/molxK	700.78	Joback Method

dvisc	0.0036492	Paxs	287.01	Joback Method
dvisc	0.0018279	Paxs	324.53	Joback Method
dvisc	0.0010567	Paxs	362.06	Joback Method
dvisc	0.0006771	Paxs	399.58	Joback Method
dvisc	0.0004683	Paxs	437.11	Joback Method
dvisc	0.0003434	Paxs	474.63	Joback Method
dvisc	0.0002635	Paxs	512.16	Joback Method

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=C13562760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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