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

Other names:	Acetoacetic acid, allyl ester
	Allyl acetoacetate
	Allyl acetylacetate
Inchi:	InChI=1S/C7H10O3/c1-3-4-10-7(9)5-6(2)8/h3H,1,4-5H2,2H3
InchiKey:	AXLMPTNTPOWPLT-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	C=CCOC(=O)CC(C)=O
Mol. weight [g/mol]:	142.15
CAS:	1118-84-9

Physical Properties

Property code	Value	Unit	Source
gf	-266.94	kJ/mol	Joback Method
hf	-419.76	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	46.41	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.695		Crippen Method
mcvol	114.200	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	486.40	K	Joback Method
tc	677.00	K	Joback Method
tf	288.98	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.50	J/mol×K	486.40	Joback Method
cpg	248.34	J/mol×K	518.17	Joback Method
cpg	257.76	J/mol×K	549.93	Joback Method
cpg	266.77	J/mol×K	581.70	Joback Method
cpg	275.37	J/mol×K	613.47	Joback Method
cpg	283.57	J/mol×K	645.24	Joback Method

cpg	291.36	J/mol×K	677.00	Joback Method
dvisc	0.0025463	Pa×s	288.98	Joback Method
dvisc	0.0014879	Pa×s	321.88	Joback Method
dvisc	0.0009605	Pa×s	354.79	Joback Method
dvisc	0.0006679	Pa×s	387.69	Joback Method
dvisc	0.0004916	Pa×s	420.59	Joback Method
dvisc	0.0003783	Pa×s	453.50	Joback Method
dvisc	0.0003016	Pa×s	486.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	467.70	K	98.30	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=C1118849&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
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume