Butanoic acid, 3-oxo-, propyl ester

Other names:	Acetoacetic acid, propyl ester
	Propyl acetoacetate
	Acetoacetic acid n-propyl ester
	Propyl ester of 3-oxobutanoic acid
Inchi:	InChI=1S/C7H12O3/c1-3-4-10-7(9)5-6(2)8/h3-5H2,1-2H3
InchiKey:	DHGFMVMDBNLMKT-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	CCCOC(=O)CC(C)=O
Mol. weight [g/mol]:	144.17
CAS:	1779-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-354.78	kJ/mol	Joback Method
hf	-545.19	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.919		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	467.00	K	NIST Webbook
tc	676.50	K	Joback Method
tf	290.74	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.79	J/mol×K	489.72	Joback Method
cpg	266.32	J/mol×K	520.85	Joback Method
cpg	276.45	J/mol×K	551.98	Joback Method
cpg	286.16	J/mol×K	583.11	Joback Method
cpg	295.47	J/mol×K	614.24	Joback Method

cpg	304.37	J/mol×K	645.37	Joback Method
cpg	312.87	J/mol×K	676.50	Joback Method
dvisc	0.0027292	Pa×s	290.74	Joback Method
dvisc	0.0015623	Pa×s	323.90	Joback Method
dvisc	0.0009920	Pa×s	357.07	Joback Method
dvisc	0.0006804	Pa×s	390.23	Joback Method
dvisc	0.0004951	Pa×s	423.39	Joback Method
dvisc	0.0003773	Pa×s	456.56	Joback Method
dvisc	0.0002983	Pa×s	489.72	Joback Method

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=C1779608&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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