Ethyl 2,4-dioxovalerate

Other names:	Ethyl acetopyruvate
	Pentanoic acid, 2,4-dioxo-, ethyl ester
Inchi:	InChI=1S/C7H10O4/c1-3-11-7(10)6(9)4-5(2)8/h3-4H2,1-2H3
InchiKey:	OYQVQWIASIXXRT-UHFFFAOYSA-N
Formula:	C7H10O4
SMILES:	CCOC(=O)C(=O)CC(C)=O
Mol. weight [g/mol]:	158.15
CAS:	615-79-2

Physical Properties

Property code	Value	Unit	Source
gf	-483.70	kJ/mol	Joback Method
hf	-657.77	kJ/mol	Joback Method
hfus	19.87	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-0.18		Crippen Method
logp	0.098		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	543.59	K	Joback Method
tc	739.40	K	Joback Method
tf	340.67	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.97	J/mol×K	543.59	Joback Method
cpg	279.75	J/mol×K	576.22	Joback Method
cpg	289.09	J/mol×K	608.86	Joback Method
cpg	297.99	J/mol×K	641.49	Joback Method
cpg	306.45	J/mol×K	674.13	Joback Method
cpg	314.45	J/mol×K	706.76	Joback Method
cpg	322.01	J/mol×K	739.40	Joback Method

dvisc	0.0023863	Pa×s	340.67	Joback Method
dvisc	0.0014690	Pa×s	374.49	Joback Method
dvisc	0.0009799	Pa×s	408.31	Joback Method
dvisc	0.0006955	Pa×s	442.13	Joback Method
dvisc	0.0005183	Pa×s	475.95	Joback Method
dvisc	0.0004016	Pa×s	509.77	Joback Method
dvisc	0.0003212	Pa×s	543.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.20	K	1.60	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615792&Units=SI

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