Ethyl trimethylacetopyruvate

Other names: Ethyl trimethylacetopyruvate
ethyl 5,5-dimethyl-2,4-dioxohexanoate
Inchi: InChI=1S/C10H16O4/c1-5-14-9(13)7(11)6-8(12)10(2,3)4/h5-6H2,1-4H3
InchiKey: NIMKIMUBJFWPTD-UHFFFAOYSA-N
Formula: C10H16O4
SMILES: CCOC(=O)C(=O)CC(=O)C(C)(C)C
Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
hf	-782.01	kJ/mol	Cheméo Relay (1.0)
hfus	20.23	kJ/mol	Joback Method
hvap	64.32	kJ/mol	Cheméo Relay (1.0)
ie	9.03	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.124		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
tb	502.50	K	Cheméo Relay (1.0)
tc	686.33	K	Cheméo Relay (1.0)
tf	318.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.19	J/mol×K	609.00	Joback Method
cpg	425.13	J/mol×K	642.13	Joback Method
cpg	437.33	J/mol×K	675.26	Joback Method
cpg	448.82	J/mol×K	708.40	Joback Method
cpg	459.61	J/mol×K	741.53	Joback Method
cpg	469.72	J/mol×K	774.66	Joback Method
cpg	479.18	J/mol×K	807.79	Joback Method
dvisc	0.0023301	Pa×s	376.90	Joback Method
dvisc	0.0013031	Pa×s	415.58	Joback Method

dvisc	0.0008046	Pa×s	454.27	Joback Method
dvisc	0.0005358	Pa×s	492.95	Joback Method
dvisc	0.0003786	Pa×s	531.63	Joback Method
dvisc	0.0002804	Pa×s	570.32	Joback Method
dvisc	0.0002157	Pa×s	609.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13395363&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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