2,2,4-Trimethyl-3-oxovaleric acid, isopropyl ester

Inchi: InChI=1S/C11H20O3/c1-7(2)9(12)11(5,6)10(13)14-8(3)4/h7-8H,1-6H3
InchiKey: YXEZWCORRAYTTO-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CC(C)OC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]: 200.27
CAS: 4337-62-6

Physical Properties

Property code	Value	Unit	Source
gf	-323.14	kJ/mol	Joback Method
hf	-647.06	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.189		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
tb	577.13	K	Joback Method
tc	773.36	K	Joback Method
tf	308.24	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.57	J/mol×K	577.13	Joback Method
cpg	512.06	J/mol×K	740.66	Joback Method
cpg	499.73	J/mol×K	707.95	Joback Method
cpg	486.64	J/mol×K	675.25	Joback Method
cpg	472.76	J/mol×K	642.54	Joback Method
cpg	458.08	J/mol×K	609.84	Joback Method
cpg	523.66	J/mol×K	773.36	Joback Method
dvisc	0.0001706	Pa×s	577.13	Joback Method
dvisc	0.0002378	Pa×s	532.32	Joback Method

dvisc	0.0003524	Pa×s	487.50	Joback Method
dvisc	0.0005654	Pa×s	442.69	Joback Method
dvisc	0.0010091	Pa×s	397.87	Joback Method
dvisc	0.0020864	Pa×s	353.06	Joback Method
dvisc	0.0053285	Pa×s	308.24	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=C4337626&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