Valeric acid, 2,2,4-trimethyl-3-oxo-, iso-butyl ester

Inchi: InChI=1S/C12H22O3/c1-8(2)7-15-11(14)12(5,6)10(13)9(3)4/h8-9H,7H2,1-6H3
InchiKey: BUGVTLLBUODWQN-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: CC(C)COC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]: 214.30
CAS: 4447-74-9

Physical Properties

Property code	Value	Unit	Source
gf	-314.72	kJ/mol	Joback Method
hf	-667.70	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	56.14	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.437		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
tb	600.01	K	Joback Method
tc	793.72	K	Joback Method
tf	319.51	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.59	J/mol×K	600.01	Joback Method
cpg	508.67	J/mol×K	632.30	Joback Method
cpg	523.89	J/mol×K	664.58	Joback Method
cpg	538.28	J/mol×K	696.87	Joback Method
cpg	551.86	J/mol×K	729.15	Joback Method
cpg	564.65	J/mol×K	761.44	Joback Method
cpg	576.69	J/mol×K	793.72	Joback Method
dvisc	0.0048352	Pa×s	319.51	Joback Method
dvisc	0.0018752	Pa×s	366.26	Joback Method

dvisc	0.0009012	Pa×s	413.01	Joback Method
dvisc	0.0005027	Pa×s	459.76	Joback Method
dvisc	0.0003123	Pa×s	506.51	Joback Method
dvisc	0.0002103	Pa×s	553.26	Joback Method
dvisc	0.0001506	Pa×s	600.01	Joback Method

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=C4447749&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume