

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

Inchi:	InChI=1S/C10H18O3/c1-6-13-9(12)10(4,5)8(11)7(2)3/h7H,6H2,1-5H3
InchiKey:	IINVHMMMAUHNDG-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCOC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]:	186.25
CAS:	4447-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-329.12	kJ/mol	Joback Method
hf	-621.14	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	52.07	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.801		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
tb	554.69	K	Joback Method
tc	749.62	K	Joback Method
tf	311.97	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.82	J/molxK	554.69	Joback Method
cpg	408.31	J/molxK	587.18	Joback Method
cpg	422.04	J/molxK	619.67	Joback Method
cpg	435.03	J/molxK	652.15	Joback Method
cpg	447.31	J/molxK	684.64	Joback Method
cpg	458.90	J/molxK	717.13	Joback Method
cpg	469.81	J/molxK	749.62	Joback Method
dvisc	0.0041458	Paxs	311.97	Joback Method
dvisc	0.0018831	Paxs	352.42	Joback Method

dvisc	0.0010063	Paxs	392.88	Joback Method
dvisc	0.0006045	Paxs	433.33	Joback Method
dvisc	0.0003961	Paxs	473.78	Joback Method
dvisc	0.0002774	Paxs	514.24	Joback Method
dvisc	0.0002047	Paxs	554.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4447647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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