

Valeric acid, 2,2,4-trimethyl-3-oxo-, methyl ester

Inchi:	InChI=1S/C9H16O3/c1-6(2)7(10)9(3,4)8(11)12-5/h6H,1-5H3
InchiKey:	FDKLXJMFRRMSQAA-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	COC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]:	172.22
CAS:	918-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-337.54	kJ/mol	Joback Method
hf	-600.50	kJ/mol	Joback Method
hfus	12.52	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.411		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	531.81	K	Joback Method
tc	729.38	K	Joback Method
tf	300.70	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.13	J/molxK	531.81	Joback Method
cpg	408.72	J/molxK	696.45	Joback Method
cpg	397.76	J/molxK	663.52	Joback Method
cpg	386.14	J/molxK	630.59	Joback Method
cpg	373.85	J/molxK	597.67	Joback Method
cpg	360.85	J/molxK	564.74	Joback Method
cpg	419.03	J/molxK	729.38	Joback Method
dvisc	0.0002285	Paxs	531.81	Joback Method
dvisc	0.0003087	Paxs	493.29	Joback Method

dvisc	0.0004390	Paxs	454.77	Joback Method
dvisc	0.0006664	Paxs	416.25	Joback Method
dvisc	0.0011013	Paxs	377.74	Joback Method
dvisc	0.0020400	Paxs	339.22	Joback Method
dvisc	0.0044253	Paxs	300.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C918718&Units=SI
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

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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