

Pentanoic acid, 2,2-dimethyl-, ethyl ester

Inchi:	InChI=1S/C9H18O2/c1-5-7-9(3,4)8(10)11-6-2/h5-7H2,1-4H3
InchiKey:	XZQBNCXOWSIKEK-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCC(C)(C)C(=O)OCC
Mol. weight [g/mol]:	158.24
CAS:	5837-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-206.18	kJ/mol	Joback Method
hf	-482.64	kJ/mol	Joback Method
hfus	14.44	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
tb	478.38	K	Joback Method
tc	662.57	K	Joback Method
tf	265.77	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.67	J/molxK	478.38	Joback Method
cpg	340.03	J/molxK	509.08	Joback Method
cpg	353.74	J/molxK	539.78	Joback Method
cpg	366.81	J/molxK	570.48	Joback Method
cpg	379.26	J/molxK	601.18	Joback Method
cpg	391.10	J/molxK	631.87	Joback Method
cpg	402.36	J/molxK	662.57	Joback Method
dvisc	0.0045510	Paxs	265.77	Joback Method
dvisc	0.0020820	Paxs	301.20	Joback Method

dvisc	0.0011229	Paxs	336.64	Joback Method
dvisc	0.0006812	Paxs	372.07	Joback Method
dvisc	0.0004508	Paxs	407.51	Joback Method
dvisc	0.0003187	Paxs	442.94	Joback Method
dvisc	0.0002372	Paxs	478.38	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=C5837934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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