Pentanoic acid, 2-ethyl-2-methyl-, methyl ester

Other names: Methyl «alpha»-ethyl-«alpha»-methylvalerate
Inchi: InChI=1S/C9H18O2/c1-5-7-9(3,6-2)8(10)11-4/h5-7H2,1-4H3
InchiKey: JVBYMEHKMMCQBG-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCC(C)(CC)C(=O)OC
Mol. weight [g/mol]: 158.24
CAS: 37974-23-5

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
rinpol	948.00		NIST Webbook
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/mol×K	478.38	Joback Method
cpg	391.10	J/mol×K	631.87	Joback Method
cpg	379.26	J/mol×K	601.18	Joback Method
cpg	366.81	J/mol×K	570.48	Joback Method
cpg	353.74	J/mol×K	539.78	Joback Method
cpg	340.03	J/mol×K	509.08	Joback Method
cpg	402.36	J/mol×K	662.57	Joback Method

dvisc	0.0002372	Pa×s	478.38	Joback Method
dvisc	0.0003187	Pa×s	442.94	Joback Method
dvisc	0.0004508	Pa×s	407.51	Joback Method
dvisc	0.0006812	Pa×s	372.07	Joback Method
dvisc	0.0011229	Pa×s	336.64	Joback Method
dvisc	0.0020820	Pa×s	301.20	Joback Method
dvisc	0.0045510	Pa×s	265.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37974235&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume