4-Pentenoic acid, 2-methyl-, 4-methyl-2-pentyl ester

Inchi: InChI=1S/C12H22O2/c1-6-7-10(4)12(13)14-11(5)8-9(2)3/h6,9-11H,1,7-8H2,2-5H3
InchiKey: PWISOICVELVVDM-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=CCC(C)C(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-103.24	kJ/mol	Joback Method
hf	-426.22	kJ/mol	Joback Method
hfus	17.77	kJ/mol	Joback Method
hvap	49.63	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.176		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	545.61	K	Joback Method
tc	728.30	K	Joback Method
tf	250.40	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.18	J/mol×K	545.61	Joback Method
cpg	461.40	J/mol×K	576.06	Joback Method
cpg	476.91	J/mol×K	606.51	Joback Method
cpg	491.71	J/mol×K	636.96	Joback Method
cpg	505.82	J/mol×K	667.40	Joback Method
cpg	519.26	J/mol×K	697.85	Joback Method
cpg	532.03	J/mol×K	728.30	Joback Method
dvisc	0.0088592	Pa×s	250.40	Joback Method

dvisc	0.0026211	Pa×s	299.60	Joback Method
dvisc	0.0010934	Pa×s	348.80	Joback Method
dvisc	0.0005662	Pa×s	398.00	Joback Method
dvisc	0.0003389	Pa×s	447.21	Joback Method
dvisc	0.0002245	Pa×s	496.41	Joback Method
dvisc	0.0001603	Pa×s	545.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406108&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