4-Pentenoic acid, 3-methyl-, methyl ester

Other names: methyl 3-methyl-4-pentenoate
Inchi: InChI=1S/C7H12O2/c1-4-6(2)5-7(8)9-3/h4,6H,1,5H2,2-3H3
InchiKey: LPKNFPRCXZELLI-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: C=CC(C)CC(=O)OC
Mol. weight [g/mol]: 128.17
CAS: 20459-97-6

Physical Properties

Property code	Value	Unit	Source
gf	-140.46	kJ/mol	Joback Method
hf	-312.46	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.372		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
ripol	1140.00		NIST Webbook
tb	432.09	K	Joback Method
tc	616.21	K	Joback Method
tf	224.05	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.93	J/mol×K	432.09	Joback Method
cpg	233.73	J/mol×K	462.78	Joback Method
cpg	244.12	J/mol×K	493.46	Joback Method
cpg	254.10	J/mol×K	524.15	Joback Method
cpg	263.67	J/mol×K	554.84	Joback Method
cpg	272.85	J/mol×K	585.52	Joback Method
cpg	281.64	J/mol×K	616.21	Joback Method

dvisc	0.0042260	Pa×s	224.05	Joback Method
dvisc	0.0019297	Pa×s	258.72	Joback Method
dvisc	0.0010605	Pa×s	293.40	Joback Method
dvisc	0.0006615	Pa×s	328.07	Joback Method
dvisc	0.0004515	Pa×s	362.74	Joback Method
dvisc	0.0003294	Pa×s	397.42	Joback Method
dvisc	0.0002529	Pa×s	432.09	Joback Method

Sources

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=C20459976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume