2-Pentenoic acid, 3-methyl-, methyl ester

Other names:	Methyl 3-methyl-2-pentenoate
Inchi:	InChI=1S/C7H12O2/c1-4-6(2)5-7(8)9-3/h5H,4H2,1-3H3/b6-5+
InchiKey:	SLQFYMAWZYTVFZ-AATRIKPKSA-N
Formula:	C7H12O2
SMILES:	CCC(C)=CC(=O)OC
Mol. weight [g/mol]:	128.17
CAS:	50652-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-154.19	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1262.00		NIST Webbook
tb	439.89	K	Joback Method
tc	628.49	K	Joback Method
tf	221.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.62	J/mol×K	439.89	Joback Method
cpg	233.55	J/mol×K	471.32	Joback Method
cpg	244.02	J/mol×K	502.76	Joback Method

cpg	254.05	J/mol×K	534.19	Joback Method
cpg	263.64	J/mol×K	565.63	Joback Method
cpg	272.80	J/mol×K	597.06	Joback Method
cpg	281.54	J/mol×K	628.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50652794&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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