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

Other names: Methyl 4-methyl-2-pentenoate
Inchi: InChI=1S/C7H12O2/c1-6(2)4-5-7(8)9-3/h4-6H,1-3H3/b5-4+
InchiKey: YVOAQDZUARKSRL-SNAWJCMRSA-N
Formula: C7H12O2
SMILES: COC(=O)C=CC(C)C
Mol. weight [g/mol]: 128.17
CAS: 50652-78-3

Physical Properties

Property code	Value	Unit	Source
gf	-148.08	kJ/mol	Joback Method
hf	-320.67	kJ/mol	Joback Method
hfus	13.35	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.372		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
ripol	1229.00		NIST Webbook
tb	439.57	K	Joback Method
tc	628.84	K	Joback Method
tf	220.73	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.78	J/mol×K	439.57	Joback Method
cpg	233.88	J/mol×K	471.11	Joback Method
cpg	244.50	J/mol×K	502.66	Joback Method
cpg	254.66	J/mol×K	534.20	Joback Method
cpg	264.37	J/mol×K	565.75	Joback Method
cpg	273.65	J/mol×K	597.29	Joback Method
cpg	282.49	J/mol×K	628.84	Joback Method

dvisc	0.0044540	Pa×s	220.73	Joback Method
dvisc	0.0018688	Pa×s	257.20	Joback Method
dvisc	0.0009729	Pa×s	293.68	Joback Method
dvisc	0.0005850	Pa×s	330.15	Joback Method
dvisc	0.0003893	Pa×s	366.62	Joback Method
dvisc	0.0002111	Pa×s	439.57	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=C50652783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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