Pentanoic acid, 3-methyl-, methyl ester

Other names:	Valeric acid, 3-methyl-, methyl ester
	Methyl «beta»-methylvalerate
	Methyl 3-methylpentanoate
	3-Methylvaleric acid, methyl ester
Inchi:	InChI=1S/C7H14O2/c1-4-6(2)5-7(8)9-3/h6H,4-5H2,1-3H3
InchiKey:	FHASOOYJUZKVFW-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(C)CC(=O)OC
Mol. weight [g/mol]:	130.18
CAS:	2177-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	875.00		NIST Webbook
rinpol	866.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1145.00		NIST Webbook
tb	435.41	K	Joback Method
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0002542	Pa×s	435.41	Joback Method
dvisc	0.0003348	Pa×s	400.48	Joback Method
dvisc	0.0004649	Pa×s	365.54	Joback Method
dvisc	0.0006919	Pa×s	330.61	Joback Method
dvisc	0.0011312	Pa×s	295.68	Joback Method
dvisc	0.0021099	Pa×s	260.74	Joback Method
dvisc	0.0047724	Pa×s	225.81	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=C2177788&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
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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