2,4-Dimethyl-3-pentanol acetate

Other names: Acetic acid, 2,4-dimethylpent-3-yl ester
Inchi: InChI=1S/C9H18O2/c1-6(2)9(7(3)4)11-8(5)10/h6-7,9H,1-5H3
InchiKey: OXCWHEWLKNJJET-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 158.24
CAS: 84612-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-216.34	kJ/mol	Joback Method
hf	-489.73	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	43.62	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.230		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
tb	480.29	K	Joback Method
tc	665.27	K	Joback Method
tf	218.35	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.38	J/mol×K	480.29	Joback Method
cpg	337.72	J/mol×K	511.12	Joback Method
cpg	351.50	J/mol×K	541.95	Joback Method
cpg	364.71	J/mol×K	572.78	Joback Method
cpg	377.36	J/mol×K	603.61	Joback Method
cpg	389.47	J/mol×K	634.44	Joback Method

cpg	401.02	J/mol×K	665.27	Joback Method
dvisc	0.0122928	Pa×s	218.35	Joback Method
dvisc	0.0035177	Pa×s	262.01	Joback Method
dvisc	0.0014391	Pa×s	305.66	Joback Method
dvisc	0.0007361	Pa×s	349.32	Joback Method
dvisc	0.0004370	Pa×s	392.98	Joback Method
dvisc	0.0002879	Pa×s	436.63	Joback Method
dvisc	0.0002047	Pa×s	480.29	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=C84612748&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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