3-Pentyl acetate

Other names: 3-Pentanol, acetate
1-ethylpropyl ethanoate
Inchi: InChI=1S/C7H14O2/c1-4-7(5-2)9-6(3)8/h7H,4-5H2,1-3H3
InchiKey: PBKYSIMDORTIEU-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCC(CC)OC(C)=O
Mol. weight [g/mol]: 130.18
CAS: 620-11-1

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	-1.73		Crippen Method
logp	1.738		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	835.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	785.00		NIST Webbook
ripol	1077.00		NIST Webbook
tb	407.00 ± 2.00	K	NIST Webbook
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=C620111&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