2-Heptanol, acetate

Other names: 1-Methylhexyl acetate
2-Heptyl acetate
Acetic acid, hept-2-yl ester
Inchi: InChI=1S/C9H18O2/c1-4-5-6-7-8(2)11-9(3)10/h8H,4-7H2,1-3H3
InchiKey: VJYWBLDDQZIGJI-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCCCC(C)OC(C)=O
Mol. weight [g/mol]: 158.24
CAS: 5921-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1022.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1021.00		NIST Webbook
ripol	1266.00		NIST Webbook

ripol	1266.00		NIST Webbook
ripol	1255.00		NIST Webbook
ripol	1255.00		NIST Webbook
ripol	1250.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53108e+01
Coeff. B	-4.15613e+03
Coeff. C	-6.77930e+01
Temperature range (K), min.	344.44
Temperature range (K), max.	483.43

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=C5921824&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor 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