2-Heptanol, 6-methyl, acetate

Other names: 1,5-dimethylhexyl acetate
Inchi: InChI=1S/C10H20O2/c1-8(2)6-5-7-9(3)12-10(4)11/h8-9H,5-7H2,1-4H3
InchiKey: JNRDWRMJYGDQQE-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CC(=O)OC(C)CCCC(C)C
Mol. weight [g/mol]: 172.26
CAS: 67952-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-205.48	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.764		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1080.00		NIST Webbook
ripol	1300.00		NIST Webbook
tb	503.61	K	Joback Method
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.51	J/mol×K	503.61	Joback Method
cpg	437.08	J/mol×K	653.07	Joback Method
cpg	424.51	J/mol×K	623.18	Joback Method
cpg	411.38	J/mol×K	593.28	Joback Method
cpg	397.67	J/mol×K	563.39	Joback Method
cpg	383.39	J/mol×K	533.50	Joback Method

cpg	449.08	J/mol×K	682.96	Joback Method
dvisc	0.0001994	Pa×s	503.61	Joback Method
dvisc	0.0002734	Pa×s	460.44	Joback Method
dvisc	0.0004002	Pa×s	417.28	Joback Method
dvisc	0.0006396	Pa×s	374.12	Joback Method
dvisc	0.0011553	Pa×s	330.95	Joback Method
dvisc	0.0024917	Pa×s	287.79	Joback Method
dvisc	0.0070487	Pa×s	244.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39901e+01
Coeff. B	-3.81132e+03
Coeff. C	-6.90720e+01
Temperature range (K), min.	347.22
Temperature range (K), max.	508.24

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67952572&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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