4-Heptanol, 2,6-dimethyl-, acetate

Other names: Diisobutylcarbinyl acetate
2,6-Dimethylheptyl-4-acetate
3-Methyl-1-isobutylbutyl acetate
Inchi: InChI=1S/C11H22O2/c1-8(2)6-11(7-9(3)4)13-10(5)12/h8-9,11H,6-7H2,1-5H3
InchiKey: XLJDNKNPKUBQMX-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CC(=O)OC(CC(C)C)CC(C)C
Mol. weight [g/mol]: 186.29
CAS: 10250-45-0

Physical Properties

Property code	Value	Unit	Source
gf	-199.50	kJ/mol	Joback Method
hf	-531.01	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	3.010		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1092.00		NIST Webbook
ripol	1265.00		NIST Webbook
tb	526.05	K	Joback Method
tc	707.25	K	Joback Method
tf	240.89	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.95	J/mol×K	526.05	Joback Method
cpg	489.63	J/mol×K	677.05	Joback Method
cpg	476.18	J/mol×K	646.85	Joback Method
cpg	462.10	J/mol×K	616.65	Joback Method

cpg	447.38	J/mol×K	586.45	Joback Method
cpg	432.00	J/mol×K	556.25	Joback Method
cpg	502.44	J/mol×K	707.25	Joback Method
dvisc	0.0001720	Pa×s	526.05	Joback Method
dvisc	0.0002429	Pa×s	478.52	Joback Method
dvisc	0.0003702	Pa×s	431.00	Joback Method
dvisc	0.0006262	Pa×s	383.47	Joback Method
dvisc	0.0012291	Pa×s	335.94	Joback Method
dvisc	0.0030130	Pa×s	288.42	Joback Method
dvisc	0.0105209	Pa×s	240.89	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C10250450&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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