1-Hexanol, 5-methyl-2-(1-methylethyl)-, acetate

Other names:	2-Isopropyl-5-methylhexyl acetate
	Tetrahydrolavandulyl acetate
	1-Hexanol, 2-isopropyl-5-methyl-, acetate
Inchi:	InChI=1S/C12H24O2/c1-9(2)6-7-12(10(3)4)8-14-11(5)13/h9-10,12H,6-8H2,1-5H3
InchiKey:	QLFSGYMLVZGFJT-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CC(=O)OCC(CCC(C)C)C(C)C
Mol. weight [g/mol]:	200.32
CAS:	40853-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-191.08	kJ/mol	Joback Method
hf	-551.65	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	50.30	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	3.258		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
tb	548.93	K	Joback Method
tc	728.36	K	Joback Method
tf	252.16	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.98	J/mol×K	548.93	Joback Method
cpg	541.73	J/mol×K	698.45	Joback Method
cpg	527.75	J/mol×K	668.55	Joback Method
cpg	513.09	J/mol×K	638.64	Joback Method
cpg	497.75	J/mol×K	608.74	Joback Method
cpg	481.72	J/mol×K	578.83	Joback Method

cpg	555.06	J/mol×K	728.36	Joback Method
dvisc	0.0001557	Pa×s	548.93	Joback Method
dvisc	0.0002202	Pa×s	499.47	Joback Method
dvisc	0.0003362	Pa×s	450.01	Joback Method
dvisc	0.0005697	Pa×s	400.54	Joback Method
dvisc	0.0011201	Pa×s	351.08	Joback Method
dvisc	0.0027490	Pa×s	301.62	Joback Method
dvisc	0.0095948	Pa×s	252.16	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=C40853552&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume