3-Octanol, 2,6-dimethyl-, acetate

Other names: 2,6-Dimethyl-3-octylacetate
Inchi: InChI=1S/C12H24O2/c1-6-10(4)7-8-12(9(2)3)14-11(5)13/h9-10,12H,6-8H2,1-5H3
InchiKey: JEBRLPRSVRFFNS-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCC(C)CCC(OC(C)=O)C(C)C
Mol. weight [g/mol]: 200.32
CAS: 123232-57-5

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	-3.34		Crippen Method
logp	3.400		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	1372.00		NIST Webbook
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	481.72	J/mol×K	578.83	Joback Method
cpg	497.75	J/mol×K	608.74	Joback Method
cpg	513.09	J/mol×K	638.64	Joback Method
cpg	527.75	J/mol×K	668.55	Joback Method
cpg	541.73	J/mol×K	698.45	Joback Method
cpg	555.06	J/mol×K	728.36	Joback Method

dvisc	0.0095948	Pa×s	252.16	Joback Method
dvisc	0.0027490	Pa×s	301.62	Joback Method
dvisc	0.0011201	Pa×s	351.08	Joback Method
dvisc	0.0005697	Pa×s	400.54	Joback Method
dvisc	0.0003362	Pa×s	450.01	Joback Method
dvisc	0.0002202	Pa×s	499.47	Joback Method
dvisc	0.0001557	Pa×s	548.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123232575&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume