3-Octanol, 3,7-dimethyl-, acetate

Other names:	Tetrahydrolinalyl acetate
	3,7-dimethyloctan-3-yl acetate
Inchi:	InChI=1S/C12H24O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h10H,6-9H2,1-5H3
InchiKey:	RBKRCARRXLFUGJ-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCC(C)(CCCC(C)C)OC(C)=O
Mol. weight [g/mol]:	200.32
CAS:	20780-48-7

Physical Properties

Property code	Value	Unit	Source
gf	-183.36	kJ/mol	Joback Method
hf	-549.84	kJ/mol	Joback Method
hfus	18.69	kJ/mol	Joback Method
hvap	49.78	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.545		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1221.10		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1224.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1438.00		NIST Webbook
tb	546.58	K	Joback Method
tc	728.79	K	Joback Method
tf	284.58	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.33	J/mol×K	546.58	Joback Method

cpg	484.29	J/mol×K	576.95	Joback Method
cpg	500.46	J/mol×K	607.32	Joback Method
cpg	515.84	J/mol×K	637.68	Joback Method
cpg	530.48	J/mol×K	668.05	Joback Method
cpg	544.39	J/mol×K	698.42	Joback Method
cpg	557.59	J/mol×K	728.79	Joback Method
dvisc	0.0055085	Pa×s	284.58	Joback Method
dvisc	0.0020765	Pa×s	328.25	Joback Method
dvisc	0.0009843	Pa×s	371.91	Joback Method
dvisc	0.0005458	Pa×s	415.58	Joback Method
dvisc	0.0003386	Pa×s	459.25	Joback Method
dvisc	0.0002282	Pa×s	502.91	Joback Method
dvisc	0.0001638	Pa×s	546.58	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20780487&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

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