3,7-Dimethyloctyl acetate

Other names:	1-Octanol, 3,7-dimethyl-, acetate
	3,7-Dimethyl-1-octanol, acetate
	3,7-Dimethyloctanyl acetate
	3,7-dimethyl-1-octyl acetate
	Dihydrocitronellyl acetate
	Tetrahydrogeranyl acetate
Inchi:	InChI=1S/C12H24O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h10-11H,5-9H2,1-4H3
InchiKey:	XFPXWDJICXBWRU-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	200.32
CAS:	20780-49-8

Physical Properties

Property code	Value	Unit	Source
gf	-188.64	kJ/mol	Joback Method
hf	-546.37	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.402		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1319.90		NIST Webbook
rinpol	1313.70		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1319.90		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1313.70		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1582.00		NIST Webbook
tb	549.37	K	Joback Method
tc	725.46	K	Joback Method
tf	267.16	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.71	J/mol×K	549.37	Joback Method
cpg	539.94	J/mol×K	696.11	Joback Method
cpg	526.20	J/mol×K	666.76	Joback Method
cpg	511.82	J/mol×K	637.42	Joback Method
cpg	496.78	J/mol×K	608.07	Joback Method
cpg	481.08	J/mol×K	578.72	Joback Method
cpg	553.06	J/mol×K	725.46	Joback Method
dvisc	0.0001657	Pa×s	549.37	Joback Method
dvisc	0.0002285	Pa×s	502.33	Joback Method
dvisc	0.0003366	Pa×s	455.30	Joback Method
dvisc	0.0005423	Pa×s	408.26	Joback Method
dvisc	0.0009890	Pa×s	361.23	Joback Method
dvisc	0.0021594	Pa×s	314.19	Joback Method
dvisc	0.0062070	Pa×s	267.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50951e+01
Coeff. B	-4.49531e+03
Coeff. C	-8.21380e+01
Temperature range (K), min.	385.72
Temperature range (K), max.	541.61

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20780498&Units=SI

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