

6-Octen-1-ol, 3,7-dimethyl-, acetate

Other names:	(.+-.)-citronellyl acetate 1-Acetoxy-3,7-dimethyloct-6-ene 2-Octen-8-ol, 2,6-dimethyl-, acetate 3,7-Dimethyl-6-octen-1-yl acetate 3,7-Dimethyl-6-octenyl acetate 6-Octen-1-ol, 3,7-dimethyl-, 1-acetate Acetic acid, 3,7-dimethyl-6-octen-1-yl ester Acetic acid, citronellyl ester Acetic acid, rhodinyll ester Cephreine Citronellol acetate Citronellyl acetate Citronellyl acetate Cytronellyl acetate NSC 4893 Natural rhodinol, acetylated dl-citronellol acetate «beta»-Citronellol, acetate «beta»-Citronellyl acetate Â«betaÂ»-Citronellol, acetate Â«betaÂ»-Citronellyl acetate
Inchi:	InChI=1S/C12H22O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h6,11H,5,7-9H2,1-4H3
InchiKey:	JOZKFWLRHCDGJA-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	198.30
CAS:	150-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-114.53	kJ/mol	Joback Method
hf	-433.66	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.322		Crippen Method

mcvol	183.080	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
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tb	553.85	K	Joback Method
tc	736.57	K	Joback Method
tf	263.12	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.19	J/mol×K	675.66	Joback Method
cpg	518.34	J/mol×K	706.11	Joback Method
cpg	445.83	J/mol×K	553.85	Joback Method
cpg	461.72	J/mol×K	584.30	Joback Method
cpg	476.90	J/mol×K	614.76	Joback Method
cpg	491.38	J/mol×K	645.21	Joback Method
cpg	530.86	J/mol×K	736.57	Joback Method
hvapt	67.80	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography
hvapt	68.70	kJ/mol	418.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41991e+01
Coeff. B	-4.19673e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	382.42
Temperature range (K), max.	552.94

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=C150845&Units=SI
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
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
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

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