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

Other names:	6-Octen-1-ol, 3,7-dimethyl-, propionate
	Citronellyl n-proprionate
	Citronellyl propanoate
	Citronellyl propianoate
	Citronellyl propionate
Inchi:	InChI=1S/C13H24O2/c1-5-13(14)15-10-9-12(4)8-6-7-11(2)3/h7,12H,5-6,8-10H2,1-4H3
InchiKey:	POPNTVRHTZDEBW-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	CCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	212.33
CAS:	141-14-0

Physical Properties

Property code	Value	Unit	Source
gf	-106.11	kJ/mol	Joback Method
hf	-454.30	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.712		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1424.70		NIST Webbook
rinpol	1445.30		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1424.70		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1445.30		NIST Webbook

rinpol	1444.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1445.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1736.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1736.00		NIST Webbook
tb	576.73	K	Joback Method
tc	757.65	K	Joback Method
tf	274.39	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.91	J/mol×K	576.73	Joback Method
cpg	512.41	J/mol×K	606.88	Joback Method
cpg	528.17	J/mol×K	637.04	Joback Method
cpg	543.21	J/mol×K	667.19	Joback Method
cpg	557.54	J/mol×K	697.35	Joback Method
cpg	571.19	J/mol×K	727.50	Joback Method
cpg	584.19	J/mol×K	757.65	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56693e+01

Coeff. B	-4.91451e+03
Coeff. C	-9.06170e+01
Temperature range (K), min.	410.12
Temperature range (K), max.	565.09

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141140&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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