Citronellyl butyrate

Other names:	2,6-Dimethyl-2-octen-8-ol, butyrate
	2,6-Dimethyl-2-octen-8-yl butyrate
	3,7-Dimethyl-6-octenyl butanoate
	3,7-Dimethyl-6-octenyl butyrate
	6-Octen-1-ol, 3,7-dimethyl-, butyrate
	Butanoic acid, 3,7-dimethyl-6-octen-1-yl ester
	Butanoic acid, 3,7-dimethyl-6-octenyl ester
	Butyric acid, 3,7-dimethyl-6-octenyl ester
	Butyric acid, ester with citronellol
	Citronellyl butanoate
	Citronellyl n-butyrate
	NSC 46147
	Natural rhodinol, butylated
	Rhodinyl butyrate
Inchi:	InChI=1S/C14H26O2/c1-5-7-14(15)16-11-10-13(4)9-6-8-12(2)3/h8,13H,5-7,9-11H2,1-4H
InchiKey:	XQPZQXTWYZAXAK-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	226.35
CAS:	141-16-2

Physical Properties

Property code	Value	Unit	Source
gf	-97.69	kJ/mol	Joback Method
hf	-474.94	kJ/mol	Joback Method
hfus	30.17	kJ/mol	Joback Method
hvap	55.56	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.102		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1531.00		NIST Webbook

rinpol	1531.00		NIST Webbook
rinpol	1531.30		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1809.00		NIST Webbook
tb	599.61	K	Joback Method
tc	778.96	K	Joback Method
tf	285.66	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.56	J/mol×K	599.61	Joback Method
cpg	564.60	J/mol×K	629.50	Joback Method

cpg	580.88	J/mol×K	659.39	Joback Method
cpg	596.40	J/mol×K	689.28	Joback Method
cpg	611.19	J/mol×K	719.17	Joback Method
cpg	625.28	J/mol×K	749.07	Joback Method
cpg	638.69	J/mol×K	778.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28805e+01
Coeff. B	-3.86144e+03
Coeff. C	-8.37640e+01
Temperature range (K), min.	390.40
Temperature range (K), max.	593.93

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=C141162&Units=SI

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