Citronellyl tiglate

Other names:	2-Butenoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester, (E)-
	3,7-Dimethyl-6-octenyl (2E)-2-methyl-2-butenoate
	E-Citronellyl tiglate
	Tiglic acid citronellyl ester
	Crotonic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester, (E)-
	3,7-Dimethyloct-6-enyl (E)-2-methylbut-2-enoate
	3,7-dimethyl-6-octenyl 2-methylcrotonate
Inchi:	InChI=1S/C15H26O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h6,8,13H,7,9-11H2,1-
InchiKey:	UCFQYMKLDPWFHZ-NSIKDUERSA-N
Formula:	C15H26O2
SMILES:	CC=C(C)C(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]:	238.37
CAS:	24717-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1670.60		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1670.60		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook

rinpol	1645.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1667.00		NIST Webbook
ripol	2010.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	2010.00		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	626.53	Joback Method
cpg	597.38	J/mol×K	657.69	Joback Method
cpg	613.87	J/mol×K	688.86	Joback Method
cpg	629.53	J/mol×K	720.02	Joback Method
cpg	644.42	J/mol×K	751.19	Joback Method
cpg	658.56	J/mol×K	782.35	Joback Method
cpg	671.98	J/mol×K	813.52	Joback Method

Sources

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=C24717859&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
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