Citronellyl hexanoate

Inchi: InChI=1S/C16H30O2/c1-5-6-7-11-16(17)18-13-12-15(4)10-8-9-14(2)3/h9,15H,5-8,10-13H
InchiKey: KNYRCCKTQMBSFP-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 254.41
CAS: 10580-25-3

Physical Properties

Property code	Value	Unit	Source
gf	-80.85	kJ/mol	Joback Method
hf	-516.22	kJ/mol	Joback Method
hfus	35.35	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.883		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1722.10		NIST Webbook
tb	645.37	K	Joback Method
tc	822.41	K	Joback Method
tf	308.20	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.22	J/mol×K	645.37	Joback Method
cpg	673.18	J/mol×K	674.88	Joback Method
cpg	690.31	J/mol×K	704.38	Joback Method
cpg	706.65	J/mol×K	733.89	Joback Method
cpg	722.20	J/mol×K	763.40	Joback Method
cpg	737.01	J/mol×K	792.90	Joback Method

cpg	751.09	J/mol×K	822.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10580253&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume