Citronellyl icosanoate

Inchi: InChI=1S/C30H58O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-30(31)32-2
InchiKey: FOLPDVUJZANDCH-UHFFFAOYSA-N
Formula: C30H58O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 450.78

Physical Properties

Property code	Value	Unit	Source
gf	37.03	kJ/mol	Joback Method
hf	-805.18	kJ/mol	Joback Method
hfus	71.61	kJ/mol	Joback Method
hvap	91.18	kJ/mol	Joback Method
log10ws	-10.85		Crippen Method
logp	10.344		Crippen Method
mcvol	436.700	ml/mol	McGowan Method
pc	629.08	kPa	Joback Method
rinpol	3118.90		NIST Webbook
rinpol	3118.90		NIST Webbook
tb	965.69	K	Joback Method
tc	1192.95	K	Joback Method
tf	465.98	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.45	J/mol×K	965.69	Joback Method
cpg	1546.55	J/mol×K	1003.57	Joback Method
cpg	1570.02	J/mol×K	1041.44	Joback Method
cpg	1591.96	J/mol×K	1079.32	Joback Method
cpg	1612.46	J/mol×K	1117.20	Joback Method
cpg	1631.65	J/mol×K	1155.08	Joback Method
cpg	1649.63	J/mol×K	1192.95	Joback Method

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=U412684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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