Citronellyl octanoate

Inchi: InChI=1S/C18H34O2/c1-5-6-7-8-9-13-18(19)20-15-14-17(4)12-10-11-16(2)3/h11,17H,5-1
InchiKey: RDBWSCQYUJLRGB-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: CCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 282.46
CAS: 72934-05-5

Physical Properties

Property code	Value	Unit	Source
gf	-64.01	kJ/mol	Joback Method
hf	-557.50	kJ/mol	Joback Method
hfus	40.53	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.663		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	1916.20		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1916.20		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	691.13	K	Joback Method
tc	867.34	K	Joback Method
tf	330.74	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.10	J/mol×K	691.13	Joback Method
cpg	786.83	J/mol×K	720.50	Joback Method
cpg	804.68	J/mol×K	749.87	Joback Method

cpg	821.68	J/mol×K	779.23	Joback Method
cpg	837.85	J/mol×K	808.60	Joback Method
cpg	853.24	J/mol×K	837.97	Joback Method
cpg	867.86	J/mol×K	867.34	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=C72934055&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume