Citronellyl isooctanoate

Inchi: InChI=1S/C18H34O2/c1-15(2)9-6-7-12-18(19)20-14-13-17(5)11-8-10-16(3)4/h10,15,17H
InchiKey: MLEVJJKUMDEYDU-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: CC(C)=CCCC(C)CCOC(=O)CCCCC(C)C
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-66.45	kJ/mol	Joback Method
hf	-562.78	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.519		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	1865.00		NIST Webbook
tb	690.69	K	Joback Method
tc	869.09	K	Joback Method
tf	315.74	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.53	J/mol×K	690.69	Joback Method
cpg	787.52	J/mol×K	720.42	Joback Method
cpg	805.60	J/mol×K	750.16	Joback Method
cpg	822.80	J/mol×K	779.89	Joback Method
cpg	839.15	J/mol×K	809.63	Joback Method
cpg	854.69	J/mol×K	839.36	Joback Method
cpg	869.43	J/mol×K	869.09	Joback Method

Sources

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=R200647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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