Citronellyl isocrotonate

Inchi: InChI=1S/C14H24O2/c1-5-7-14(15)16-11-10-13(4)9-6-8-12(2)3/h5,7-8,13H,6,9-11H2,1-4
InchiKey: MYGZJMACIRJNPL-ALCCZGGFSA-N
Formula: C14H24O2
SMILES: CC=CC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-17.47	kJ/mol	Joback Method
hf	-357.72	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.878		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1833.00		NIST Webbook
tb	603.77	K	Joback Method
tc	789.85	K	Joback Method
tf	280.58	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.76	J/mol×K	603.77	Joback Method
cpg	544.41	J/mol×K	634.78	Joback Method
cpg	560.24	J/mol×K	665.80	Joback Method
cpg	575.29	J/mol×K	696.81	Joback Method
cpg	589.60	J/mol×K	727.82	Joback Method
cpg	603.19	J/mol×K	758.84	Joback Method

cpg	616.10	J/mol×K	789.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409577&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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