(S)-(-)-Citronellic acid, methyl ester

Inchi: InChI=1S/C11H20O2/c1-9(2)6-5-7-10(3)8-11(12)13-4/h6,10H,5,7-8H2,1-4H3
InchiKey: ZFLPOPCZMXGUOJ-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: COC(=O)CC(C)CCC=C(C)C
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-122.95	kJ/mol	Joback Method
hf	-413.02	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	48.89	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
tb	530.97	K	Joback Method
tc	715.64	K	Joback Method
tf	251.85	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.44	J/mol×K	530.97	Joback Method
cpg	412.62	J/mol×K	561.75	Joback Method
cpg	427.13	J/mol×K	592.53	Joback Method
cpg	440.98	J/mol×K	623.31	Joback Method
cpg	454.19	J/mol×K	654.08	Joback Method
cpg	466.77	J/mol×K	684.86	Joback Method
cpg	478.75	J/mol×K	715.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333551&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