Citronellic acid

Other names:	Citronellic acid
	3,7-Dimethyl-6-octenoic acid
Inchi:	InChI=1S/C10H18O2/c1-8(2)5-4-6-9(3)7-10(11)12/h5,9H,4,6-7H2,1-3H3,(H,11,12)
InchiKey:	GJWSUKYXUMVMGX-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(C)=CCCC(C)CC(=O)O
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
hf	-533.56	kJ/mol	Cheméo Relay (1.0)
hfus	22.71	kJ/mol	Joback Method
hvap	83.82	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
logp	2.844		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1305.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1340.80		NIST Webbook
rinpol	1345.40		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1287.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2255.00		NIST Webbook
tb	516.66	K	Cheméo Relay (1.0)
tc	696.73	K	Cheméo Relay (1.0)
tf	276.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.37	J/mol×K	577.85	Joback Method
cpg	395.74	J/mol×K	607.65	Joback Method
cpg	407.51	J/mol×K	637.44	Joback Method
cpg	418.72	J/mol×K	667.24	Joback Method
cpg	429.37	J/mol×K	697.03	Joback Method
cpg	439.51	J/mol×K	726.83	Joback Method
cpg	449.16	J/mol×K	756.62	Joback Method
hvapt	68.70	kJ/mol	451.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502476&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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