6-Octenoic acid, 3,7-dimethyl-, methyl ester

Other names:	Methyl citronellate
	Methyl 3,7-dimethyl-6-octenoate
	Citronellic acid, methyl ester
	methyl 3,7-dimethyloct-6-enoate
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
CAS:	2270-60-2

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
rinpol	1258.00		NIST Webbook
rinpol	1262.10		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1261.00		NIST Webbook

rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1262.10		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1264.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1596.00		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

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=C2270602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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