Ethyl geranate

Other names:	2,6-Octadienoic acid, 3,7-dimethyl-, ethyl ester, (E)-
	(E)-3,7-Dimethyl-2,6-octadienoic acid, ethyl ester
	Ethyl (2E)-3,7-dimethyl-2,6-octadienoate
	E-Ethyl geranate
	Ethyl (E)-3,7-dimethylocta-2,6-dienoate
	Ethyl trans-geraniate
Inchi:	InChI=1S/C12H20O2/c1-5-14-12(13)9-11(4)8-6-7-10(2)3/h7,9H,5-6,8H2,1-4H3/b11-9+
InchiKey:	ZPKNTCZTABQJPS-PKNBQFBNSA-N
Formula:	C12H20O2
SMILES:	CCOC(=O)C=C(C)CCC=C(C)C
Mol. weight [g/mol]:	196.29
CAS:	32659-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-40.42	kJ/mol	Joback Method
hf	-320.95	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	51.54	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1347.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1762.00		NIST Webbook
tb	558.33	K	Joback Method
tc	748.06	K	Joback Method
tf	259.08	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.65	J/mol×K	558.33	Joback Method
cpg	442.01	J/mol×K	589.95	Joback Method
cpg	456.62	J/mol×K	621.57	Joback Method
cpg	470.50	J/mol×K	653.20	Joback Method
cpg	483.69	J/mol×K	684.82	Joback Method
cpg	496.22	J/mol×K	716.44	Joback Method
cpg	508.12	J/mol×K	748.06	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32659215&Units=SI

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