ethyl linalyl acetate 1

Inchi: InChI=1S/C13H24O2/c1-6-13(7-2,15-12(5)14)10-8-9-11(3)4/h9H,6-8,10H2,1-5H3
InchiKey: KVHMWAPYAFPSRE-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CCC(CC)(CCC=C(C)C)OC(C)=O
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-100.83	kJ/mol	Joback Method
hf	-457.77	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.855		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1333.90		NIST Webbook
rinpol	1316.50		NIST Webbook
rinpol	1316.50		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
tb	573.94	K	Joback Method
tc	761.04	K	Joback Method
tf	291.81	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.53	J/mol×K	573.94	Joback Method
cpg	515.55	J/mol×K	605.12	Joback Method
cpg	531.70	J/mol×K	636.31	Joback Method
cpg	547.02	J/mol×K	667.49	Joback Method

cpg	561.54	J/mol×K	698.67	Joback Method
cpg	575.30	J/mol×K	729.85	Joback Method
cpg	588.34	J/mol×K	761.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R185503&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