ethyl linalool 2

Inchi: InChI=1S/C11H22O/c1-5-11(12,6-2)9-7-8-10(3)4/h8,12H,5-7,9H2,1-4H3
InchiKey: OKANGIKHTABXMV-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCC(O)(CC)CCC=C(C)C
Mol. weight [g/mol]: 170.29

Physical Properties

Property code	Value	Unit	Source
gf	-20.57	kJ/mol	Joback Method
hf	-323.92	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	55.50	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.284		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1181.80		NIST Webbook
rinpol	1181.80		NIST Webbook
tb	544.07	K	Joback Method
tc	718.97	K	Joback Method
tf	257.93	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.20	J/mol×K	544.07	Joback Method
cpg	427.75	J/mol×K	573.22	Joback Method
cpg	441.56	J/mol×K	602.37	Joback Method
cpg	454.68	J/mol×K	631.52	Joback Method
cpg	467.14	J/mol×K	660.67	Joback Method
cpg	478.98	J/mol×K	689.82	Joback Method
cpg	490.23	J/mol×K	718.97	Joback Method

Sources

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=R185494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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