

Ethanal, ethyl linalyl acetal, # 1

Inchi:	InChI=1S/C14H26O2/c1-7-14(6,11-9-10-12(3)4)16-13(5)15-8-2/h7,10,13H,1,8-9,11H2,2-
InchiKey:	ZJPKYCLAROITRY-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	C=CC(C)(CCC=C(C)C)OC(C)OCC
Mol. weight [g/mol]:	226.35

Physical Properties

Property code	Value	Unit	Source
gf	16.91	kJ/mol	Joback Method
hf	-377.90	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.077		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1558.00		NIST Webbook
tb	561.61	K	Joback Method
tc	744.44	K	Joback Method
tf	258.62	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.49	J/molxK	561.61	Joback Method
cpg	548.77	J/molxK	592.08	Joback Method
cpg	566.17	J/molxK	622.55	Joback Method
cpg	582.72	J/molxK	653.02	Joback Method
cpg	598.46	J/molxK	683.50	Joback Method
cpg	613.41	J/molxK	713.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R409760&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
mccvol:	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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