Ethanal, citronellyl methyl acetal

Inchi: InChI=1S/C13H26O2/c1-11(2)7-6-8-12(3)9-10-15-13(4)14-5/h7,12-13H,6,8-10H2,1-5H3
InchiKey: YSABATHBMSLQLP-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: COC(C)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 214.34

Physical Properties

Property code	Value	Unit	Source
gf	-84.63	kJ/mol	Joback Method
hf	-479.22	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.768		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
tb	544.84	K	Joback Method
tc	720.13	K	Joback Method
tf	231.69	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.09	J/mol×K	544.84	Joback Method
cpg	514.67	J/mol×K	574.06	Joback Method
cpg	531.54	J/mol×K	603.27	Joback Method
cpg	547.72	J/mol×K	632.49	Joback Method
cpg	563.21	J/mol×K	661.70	Joback Method
cpg	578.05	J/mol×K	690.92	Joback Method

cpg	592.22	J/mol×K	720.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409740&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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