Citronellol, carbamate

Inchi: InChI=1S/C11H21NO2/c1-9(2)5-4-6-10(3)7-8-14-11(12)13/h5,10H,4,6-8H2,1-3H3,(H2,12
InchiKey: PIYCXVKTSFJWDD-JTQLQIEISA-N
Formula: C11H21NO2
SMILES: CC(C)=CCCC(C)CCOC(N)=O
Mol. weight [g/mol]: 199.29

Physical Properties

Property code	Value	Unit	Source
gf	-56.50	kJ/mol	Joback Method
hf	-379.23	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	59.53	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.854		Crippen Method
mcvol	178.970	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	603.50	K	Joback Method
tc	797.20	K	Joback Method
tf	335.11	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.59	J/mol×K	603.50	Joback Method
cpg	477.53	J/mol×K	635.78	Joback Method
cpg	491.72	J/mol×K	668.07	Joback Method
cpg	505.19	J/mol×K	700.35	Joback Method
cpg	517.96	J/mol×K	732.63	Joback Method
cpg	530.06	J/mol×K	764.92	Joback Method
cpg	541.51	J/mol×K	797.20	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=R579443&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