Citronellic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi: InChI=1S/C14H25NO/c1-11(2)7-6-8-12(3)9-13-15-14(4,5)10-16-13/h7,12H,6,8-10H2,1-5

InchiKey: MEMKUNKVVADDCW-UHFFFAOYSA-N

Formula: C14H25NO

SMILES: CC(C)=CCCC(C)CC1=NC(C)(C)CO1

Mol. weight [g/mol]: 223.36

Physical Properties

Property code	Value	Unit	Source
hfus	28.97	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Cheméo Relay (1.0)
logp	3.966		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
rinpol	1452.20		NIST Webbook
rinpol	1452.20		NIST Webbook
tb	525.93	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.32	J/mol×K	623.63	Joback Method
cpg	586.37	J/mol×K	659.16	Joback Method
cpg	605.34	J/mol×K	694.69	Joback Method
cpg	623.36	J/mol×K	730.22	Joback Method
cpg	640.55	J/mol×K	765.75	Joback Method
cpg	657.02	J/mol×K	801.28	Joback Method
cpg	672.91	J/mol×K	836.81	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333627&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature