(S)-(-)-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]: 223.35

Physical Properties

Property code	Value	Unit	Source
gf	218.28	kJ/mol	Joback Method
hf	-169.14	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.966		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1450.60		NIST Webbook
rinpol	1450.60		NIST Webbook
tb	623.63	K	Joback Method
tc	836.81	K	Joback Method
tf	359.69	K	Joback Method
vc	0.789	m3/kmol	Joback Method

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:	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333552&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
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

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