

(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,6,8-10H2,1-5H
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	1450.60		NIST Webbook
rinpol	1450.60		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U333552&Units=SI>
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvac:	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

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