9-Decenoic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi: InChI=1S/C14H25NO/c1-4-5-6-7-8-9-10-11-13-15-14(2,3)12-16-13/h4H,1,5-12H2,2-3H3
InchiKey: WCWKMKCASOICGI-UHFFFAOYSA-N
Formula: C14H25NO
SMILES: C=CCCCCCCCC1=NC(C)(C)CO1
Mol. weight [g/mol]: 223.36

Physical Properties

Property code	Value	Unit	Source
hfus	32.32	kJ/mol	Joback Method
logp	4.110		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
rinpol	1512.30		NIST Webbook
rinpol	1512.30		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.47	J/mol×K	616.71	Joback Method
cpg	583.68	J/mol×K	650.28	Joback Method
cpg	601.90	J/mol×K	683.85	Joback Method
cpg	619.25	J/mol×K	717.42	Joback Method
cpg	635.82	J/mol×K	750.99	Joback Method
cpg	651.69	J/mol×K	784.56	Joback Method
cpg	666.97	J/mol×K	818.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333578&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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

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