cis-10-Nonadecenoic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi: InChI=1S/C23H43NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-24-23(2,3)21

InchiKey: IDKXOHTUQXKKIK-QXMHVHEDSA-N

Formula: C23H43NO

SMILES: CCCCCCCC/C=C\CCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 349.60

Physical Properties

Property code	Value	Unit	Source
hfus	57.11	kJ/mol	Joback Method
ie	8.47	eV	Cheméo Relay (1.0)
logp	7.621		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
rinpol	2404.40		NIST Webbook
rinpol	2404.40		NIST Webbook
tb	613.74	K	Cheméo Relay (1.0)
tf	268.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.98	J/mol×K	830.11	Joback Method
cpg	1117.53	J/mol×K	862.62	Joback Method
cpg	1139.32	J/mol×K	895.13	Joback Method
cpg	1160.47	J/mol×K	927.64	Joback Method
cpg	1181.08	J/mol×K	960.15	Joback Method
cpg	1201.27	J/mol×K	992.66	Joback Method
cpg	1221.16	J/mol×K	1025.16	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=U333645&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point