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: CCCCCCCCC=CCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 349.59

Physical Properties

Property code	Value	Unit	Source
gf	305.05	kJ/mol	Joback Method
hf	-339.83	kJ/mol	Joback Method
hfus	57.11	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.621		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2404.40		NIST Webbook
rinpol	2404.40		NIST Webbook
tb	830.11	K	Joback Method
tc	1025.16	K	Joback Method
tf	490.08	K	Joback Method
vc	1.298	m3/kmol	Joback Method

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

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=U333645&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