cis-9-Octadecenoic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi: InChI=1S/C22H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23-22(2,3)20-24

InchiKey: CHAMUCPNQGNBLJ-QXMHVHEDSA-N

Formula: C22H41NO

SMILES: CCCCCCCC/C=C\CCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 335.58

Physical Properties

Property code	Value	Unit	Source
hfus	54.52	kJ/mol	Joback Method
ie	8.43	eV	Cheméo Relay (1.0)
logp	7.231		Crippen Method
mcvol	317.230	ml/mol	McGowan Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook
tb	606.97	K	Cheméo Relay (1.0)
tf	264.17	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.00	J/mol×K	807.23	Joback Method
cpg	1054.08	J/mol×K	839.57	Joback Method
cpg	1075.38	J/mol×K	871.91	Joback Method
cpg	1096.01	J/mol×K	904.26	Joback Method
cpg	1116.07	J/mol×K	936.60	Joback Method
cpg	1135.68	J/mol×K	968.94	Joback Method
cpg	1154.95	J/mol×K	1001.28	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333212&Units=SI

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