cis-5,8,11-Eicosatrienoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C24H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-25-24(2,3

InchiKey: NIUBUFUXSPHAQF-IHDWIWDKSA-N

Formula: C24H41NO

SMILES: CCCCCCCCC=CCC=CCC=CCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 359.59

Physical Properties

Property code	Value	Unit	Source
gf	473.91	kJ/mol	Joback Method
hf	-126.03	kJ/mol	Joback Method
hfus	60.11	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.563		Crippen Method
mcvol	336.810	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2468.90		NIST Webbook
tb	861.31	K	Joback Method
tc	1064.86	K	Joback Method
tf	491.19	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.13	J/mol×K	861.31	Joback Method
cpg	1129.61	J/mol×K	895.23	Joback Method
cpg	1151.54	J/mol×K	929.16	Joback Method
cpg	1173.06	J/mol×K	963.08	Joback Method
cpg	1194.34	J/mol×K	997.01	Joback Method
cpg	1215.53	J/mol×K	1030.93	Joback Method
cpg	1236.79	J/mol×K	1064.86	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=U333534&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