cis-5,8,11,14-Eicosatetraenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C24H39NO/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: ZPFSFXNCUITIAF-GKFVBPDJSA-N

Formula: C24H39NO

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

Mol. weight [g/mol]: 357.57

Physical Properties

Property code	Value	Unit	Source
gf	554.13	kJ/mol	Joback Method
hf	-8.81	kJ/mol	Joback Method
hfus	60.31	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	7.339		Crippen Method
mcvol	332.510	ml/mol	McGowan Method
pc	1056.88	kPa	Joback Method
rinpol	2464.10		NIST Webbook
rinpol	2464.10		NIST Webbook
tb	865.47	K	Joback Method
tc	1073.03	K	Joback Method
tf	486.11	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.01	J/mol×K	865.47	Joback Method
cpg	1103.26	J/mol×K	900.06	Joback Method
cpg	1125.06	J/mol×K	934.66	Joback Method
cpg	1146.58	J/mol×K	969.25	Joback Method
cpg	1168.01	J/mol×K	1003.84	Joback Method
cpg	1189.52	J/mol×K	1038.44	Joback Method
cpg	1211.29	J/mol×K	1073.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333228&Units=SI
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

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