cis, cis, cis-9, 12, 15-Octadecatrienoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C22H37NO/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: HOXFPHDQNBUELG-AGRJPVHOSA-N

Formula: C22H37NO

SMILES: CCC=CCC=CCC=CCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
gf	457.07	kJ/mol	Joback Method
hf	-84.75	kJ/mol	Joback Method
hfus	54.93	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.783		Crippen Method
mcvol	308.630	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2303.80		NIST Webbook
tb	815.55	K	Joback Method
tc	1018.58	K	Joback Method
tf	468.65	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.97	J/mol×K	815.55	Joback Method
cpg	1003.41	J/mol×K	849.39	Joback Method
cpg	1024.21	J/mol×K	883.23	Joback Method
cpg	1044.50	J/mol×K	917.06	Joback Method
cpg	1064.43	J/mol×K	950.90	Joback Method
cpg	1084.16	J/mol×K	984.74	Joback Method
cpg	1103.83	J/mol×K	1018.58	Joback Method

Sources

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=U333200&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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