cis-13,16-Docasadienoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C26H47NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27

InchiKey: YGUQQCLTZSTBIH-MURFETPASA-N

Formula: C26H47NO

SMILES: CCCCCC=CCC=CCCCCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 389.66

Physical Properties

Property code	Value	Unit	Source
gf	410.53	kJ/mol	Joback Method
hf	-284.53	kJ/mol	Joback Method
hfus	65.09	kJ/mol	Joback Method
hvap	84.17	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	8.568		Crippen Method
mcvol	369.290	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2707.00		NIST Webbook
tb	902.91	K	Joback Method
tc	1107.52	K	Joback Method
tf	518.81	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.72	J/mol×K	902.91	Joback Method
cpg	1286.84	J/mol×K	937.01	Joback Method
cpg	1310.38	J/mol×K	971.11	Joback Method
cpg	1333.49	J/mol×K	1005.22	Joback Method
cpg	1356.32	J/mol×K	1039.32	Joback Method
cpg	1379.03	J/mol×K	1073.42	Joback Method
cpg	1401.76	J/mol×K	1107.52	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=U333604&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