cis-13-Docosenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C26H49NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27

InchiKey: UWSMPEYMQYZXKM-QXMHVHEDSA-N

Formula: C26H49NO

SMILES: CCCCCCCCC=CCCCCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 391.67

Physical Properties

Property code	Value	Unit	Source
gf	330.31	kJ/mol	Joback Method
hf	-401.75	kJ/mol	Joback Method
hfus	64.88	kJ/mol	Joback Method
hvap	84.21	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.792		Crippen Method
mcvol	373.590	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	898.75	K	Joback Method
tc	1101.33	K	Joback Method
tf	523.89	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.22	J/mol×K	898.75	Joback Method
cpg	1313.66	J/mol×K	932.51	Joback Method
cpg	1337.41	J/mol×K	966.28	Joback Method
cpg	1360.59	J/mol×K	1000.04	Joback Method
cpg	1383.34	J/mol×K	1033.81	Joback Method
cpg	1405.80	J/mol×K	1067.57	Joback Method
cpg	1428.11	J/mol×K	1101.33	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=U333240&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