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

Inchi: InChI=1S/C24H45NO/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: RRQQGMJTXGRWPL-KTKRTIGZSA-N

Formula: C24H45NO

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

Mol. weight [g/mol]: 363.62

Physical Properties

Property code	Value	Unit	Source
gf	313.47	kJ/mol	Joback Method
hf	-360.47	kJ/mol	Joback Method
hfus	59.70	kJ/mol	Joback Method
hvap	79.76	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.011		Crippen Method
mcvol	345.410	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	852.99	K	Joback Method
tc	1049.76	K	Joback Method
tf	501.35	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.87	J/mol×K	852.99	Joback Method
cpg	1181.96	J/mol×K	885.79	Joback Method
cpg	1204.31	J/mol×K	918.58	Joback Method
cpg	1226.04	J/mol×K	951.38	Joback Method
cpg	1247.27	J/mol×K	984.17	Joback Method
cpg	1268.12	J/mol×K	1016.97	Joback Method
cpg	1288.71	J/mol×K	1049.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333522&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