cis-15-Tetracosenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C28H53NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25

InchiKey: JHOIBVDGYFJMIL-QXMHVHEDSA-N

Formula: C28H53NO

SMILES: CCCCCCCCC=CCCCCCCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 419.73

Physical Properties

Property code	Value	Unit	Source
gf	347.15	kJ/mol	Joback Method
hf	-443.03	kJ/mol	Joback Method
hfus	70.07	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.572		Crippen Method
mcvol	401.770	ml/mol	McGowan Method
pc	764.79	kPa	Joback Method
rinpol	2908.20		NIST Webbook
rinpol	2908.20		NIST Webbook
tb	944.51	K	Joback Method
tc	1156.50	K	Joback Method
tf	546.43	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.80	J/mol×K	944.51	Joback Method
cpg	1449.06	J/mol×K	979.84	Joback Method
cpg	1474.67	J/mol×K	1015.17	Joback Method
cpg	1499.78	J/mol×K	1050.50	Joback Method
cpg	1524.56	J/mol×K	1085.84	Joback Method
cpg	1549.18	J/mol×K	1121.17	Joback Method
cpg	1573.80	J/mol×K	1156.50	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=U333244&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