10,12-Tricosadiynoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C27H45NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26

InchiKey: LCSZIPJVAPVYFJ-UHFFFAOYSA-N

Formula: C27H45NO

SMILES: CCCCCCCCCCC#CC#CCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 399.65

Physical Properties

Property code	Value	Unit	Source
gf	664.11	kJ/mol	Joback Method
hf	4.99	kJ/mol	Joback Method
hfus	73.52	kJ/mol	Joback Method
hvap	90.78	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	7.852		Crippen Method
mcvol	374.780	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
rinpol	3006.90		NIST Webbook
rinpol	3006.90		NIST Webbook
tb	935.47	K	Joback Method
tc	1151.07	K	Joback Method
tf	752.44	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.57	J/mol×K	935.47	Joback Method
cpg	1301.73	J/mol×K	971.40	Joback Method
cpg	1325.24	J/mol×K	1007.34	Joback Method
cpg	1348.25	J/mol×K	1043.27	Joback Method
cpg	1370.90	J/mol×K	1079.20	Joback Method
cpg	1393.34	J/mol×K	1115.13	Joback Method
cpg	1415.70	J/mol×K	1151.07	Joback Method

Sources

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=U333595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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