17-Octadecynoic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi: InChI=1S/C22H39NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23-22(2,3)20-24

InchiKey: OZWNNKSXUFZEAK-UHFFFAOYSA-N

Formula: C22H39NO

SMILES: C#CCCCCCCCCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 333.56

Physical Properties

Property code	Value	Unit	Source
hfus	57.30	kJ/mol	Joback Method
logp	6.678		Crippen Method
mcvol	312.930	ml/mol	McGowan Method
rinpol	2349.60		NIST Webbook
rinpol	2349.60		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.54	J/mol×K	793.19	Joback Method
cpg	1022.19	J/mol×K	825.71	Joback Method
cpg	1043.03	J/mol×K	858.23	Joback Method
cpg	1063.17	J/mol×K	890.75	Joback Method
cpg	1082.72	J/mol×K	923.27	Joback Method
cpg	1101.78	J/mol×K	955.79	Joback Method
cpg	1120.45	J/mol×K	988.31	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333541&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices