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]: 333.55

Physical Properties

Property code	Value	Unit	Source
gf	439.48	kJ/mol	Joback Method
hf	-144.51	kJ/mol	Joback Method
hfus	57.30	kJ/mol	Joback Method
hvap	75.20	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.678		Crippen Method
mcvol	312.930	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2349.60		NIST Webbook
rinpol	2349.60		NIST Webbook
tb	793.19	K	Joback Method
tc	988.31	K	Joback Method
tf	530.86	K	Joback Method
vc	1.224	m3/kmol	Joback Method

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

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=U333541&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