cis-10-Heptadecenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C21H39NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-22-21(2,3)19-23-2(

InchiKey: HMKQVZSFQFGNGC-KTKRTIGZSA-N

Formula: C21H39NO

SMILES: CCCCCCC=CCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 321.54

Physical Properties

Property code	Value	Unit	Source
gf	288.21	kJ/mol	Joback Method
hf	-298.55	kJ/mol	Joback Method
hfus	51.94	kJ/mol	Joback Method
hvap	73.08	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.841		Crippen Method
mcvol	303.140	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2212.10		NIST Webbook
rinpol	2212.10		NIST Webbook
tb	784.35	K	Joback Method
tc	978.06	K	Joback Method
tf	467.54	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.96	J/mol×K	784.35	Joback Method
cpg	991.63	J/mol×K	816.63	Joback Method
cpg	1012.50	J/mol×K	848.92	Joback Method
cpg	1032.67	J/mol×K	881.20	Joback Method
cpg	1052.24	J/mol×K	913.49	Joback Method
cpg	1071.33	J/mol×K	945.77	Joback Method
cpg	1090.04	J/mol×K	978.06	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=U333622&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