cis-9-Hexadecenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C20H37NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-21-20(2,3)18-22-19/h9

InchiKey: BYFWBRIYEWDFSU-KTKRTIGZSA-N

Formula: C20H37NO

SMILES: CCCCCCC=CCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 307.51

Physical Properties

Property code	Value	Unit	Source
gf	279.79	kJ/mol	Joback Method
hf	-277.91	kJ/mol	Joback Method
hfus	49.34	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.451		Crippen Method
mcvol	289.050	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2104.00		NIST Webbook
rinpol	2104.00		NIST Webbook
tb	761.47	K	Joback Method
tc	955.44	K	Joback Method
tf	456.27	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.91	J/mol×K	761.47	Joback Method
cpg	930.22	J/mol×K	793.80	Joback Method
cpg	950.69	J/mol×K	826.13	Joback Method
cpg	970.44	J/mol×K	858.46	Joback Method
cpg	989.57	J/mol×K	890.78	Joback Method
cpg	1008.19	J/mol×K	923.11	Joback Method
cpg	1026.39	J/mol×K	955.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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