cis-5-Dodecenoic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi: InChI=1S/C16H29NO/c1-4-5-6-7-8-9-10-11-12-13-15-17-16(2,3)14-18-15/h9-10H,4-8,11-

InchiKey: QEHKFZIOHYDWJH-KTKRTIGZSA-N

Formula: C16H29NO

SMILES: CCCCCCC=CCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 251.41

Physical Properties

Property code	Value	Unit	Source
gf	246.11	kJ/mol	Joback Method
hf	-195.35	kJ/mol	Joback Method
hfus	38.98	kJ/mol	Joback Method
hvap	61.95	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.891		Crippen Method
mcvol	232.690	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1697.90		NIST Webbook
rinpol	1697.90		NIST Webbook
rinpol	1698.10		NIST Webbook
tb	669.95	K	Joback Method
tc	870.09	K	Joback Method
tf	411.19	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.57	J/mol×K	669.95	Joback Method
cpg	695.60	J/mol×K	703.31	Joback Method
cpg	714.69	J/mol×K	736.66	Joback Method
cpg	732.95	J/mol×K	770.02	Joback Method
cpg	750.48	J/mol×K	803.38	Joback Method
cpg	767.39	J/mol×K	836.73	Joback Method
cpg	783.77	J/mol×K	870.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333124&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

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