

Trans-13-octadecenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C22H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23-22(2,3)20-2
InchiKey: LAPZQVVNBSJZOY-BQYQJAHWSA-N
Formula: C22H41NO
SMILES: CCCC/C=C/CCCCCCCCCCCCC1=NC(C)(C)CO1
Mol. weight [g/mol]: 335.58

Physical Properties

Property code	Value	Unit	Source
hfus	54.52	kJ/mol	Joback Method
logp	7.231		Crippen Method
mcvol	317.230	ml/mol	McGowan Method
rinpol	2314.80		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.00	J/mol×K	807.23	Joback Method
cpg	1054.08	J/mol×K	839.57	Joback Method
cpg	1075.38	J/mol×K	871.91	Joback Method
cpg	1096.01	J/mol×K	904.26	Joback Method
cpg	1116.07	J/mol×K	936.60	Joback Method
cpg	1135.68	J/mol×K	968.94	Joback Method
cpg	1154.95	J/mol×K	1001.28	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333614&Units=SI>
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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

Legend

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

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