

10-Undecenoic acid, 4,4-dimethyloxazoline derivative

Other names:

10-Undecenoic acid, DMOX derivative

10-Undecenoic acid, 4,4-Dimethyloxazoline (DMOX) derivative

Inchi:

InChI=1S/C15H27NO/c1-4-5-6-7-8-9-10-11-12-14-16-15(2,3)13-17-14/h4H,1,5-13H2,2-3

InchiKey:

WMCSKOUUEEYZGDK-UHFFFAOYSA-N

Formula:

C15H27NO

SMILES:

C=CCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]:

237.38

Physical Properties

Property code	Value	Unit	Source
gf	245.31	kJ/mol	Joback Method
hf	-166.50	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	59.09	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.500		Crippen Method
mcvol	218.600	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1614.50		NIST Webbook
rinpol	1614.50		NIST Webbook
tb	639.59	K	Joback Method
tc	838.33	K	Joback Method
tf	403.24	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.38	J/molxK	639.59	Joback Method
cpg	637.96	J/molxK	672.71	Joback Method
cpg	656.59	J/molxK	705.84	Joback Method
cpg	674.35	J/molxK	738.96	Joback Method
cpg	691.35	J/molxK	772.08	Joback Method
cpg	707.68	J/molxK	805.20	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=U333568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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