

# Ethaneperoxoic acid, 1-cyano-1-[2-(2-phenyl-1,3-dioxolan-2-yl)ethyl]per

Inchi:  
ester

InChI=1S/C19H25NO5/c1-3-4-10-18(15-20,25-24-16(2)21)11-12-19(22-13-14-23-19)17-8

InchiKey:

XBNHWTBTLQIXHU-UHFFFAOYSA-N

Formula:

C19H25NO5

SMILES:

CCCCC(C#N)(CCC1(c2ccccc2)OCCO1)OOC(C)=O

Mol. weight [g/mol]:

347.41

CAS:

58422-92-7

## Physical Properties

Property code	Value	Unit	Source
gf	-122.57	kJ/mol	Joback Method
hf	-608.13	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	89.04	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.614		Crippen Method
mcvol	270.380	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
tb	927.78	K	Joback Method
tc	1160.93	K	Joback Method
tf	580.05	K	Joback Method
vc	1.030	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.19	J/molxK	927.78	Joback Method
cpg	900.26	J/molxK	966.64	Joback Method
cpg	917.02	J/molxK	1005.50	Joback Method
cpg	933.66	J/molxK	1044.35	Joback Method
cpg	950.35	J/molxK	1083.21	Joback Method
cpg	967.26	J/molxK	1122.07	Joback Method
cpg	984.58	J/molxK	1160.93	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C58422927&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58422927&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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