

5(4H)-Oxazolone, 2-phenyl-4-(phenylmethylene)-, (Z)-

Other names:

2-Oxazolin-5-one, 4-benzylidene-2-phenyl-, (Z)-

(Z)-4-Benzylidene-2-phenyloxazolin-5-one

4-Benzylidene-2-phenyl-1,3-oxazol-5(4H)-one, cis-

Inchi:

InChI=1S/C16H11NO2/c18-16-14(11-12-7-3-1-4-8-12)17-15(19-16)13-9-5-2-6-10-13/h1-

InchiKey:

VFDOKJVMHZUBTN-KAMYIIQDSA-N

Formula:

C16H11NO2

SMILES:

O=C1OC(c2ccccc2)=N/C1=C/c1ccccc1

Mol. weight [g/mol]:

249.27

Physical Properties

Property code	Value	Unit	Source
hfus	31.93	kJ/mol	Joback Method
logp	3.031		Crippen Method
mcvol	186.740	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.50	J/mol×K	798.04	Joback Method
cpg	551.87	J/mol×K	845.67	Joback Method
cpg	565.40	J/mol×K	893.30	Joback Method
cpg	577.15	J/mol×K	940.93	Joback Method
cpg	587.18	J/mol×K	988.56	Joback Method
cpg	595.56	J/mol×K	1036.19	Joback Method
cpg	602.35	J/mol×K	1083.82	Joback Method

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C17606701>

Legend

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

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