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

Other names: 2-Oxazolin-5-one, 4-benzylidene-2-phenyl-
4-Benzylidene-2-phenyl-5(4H)-oxazolone
5(4H)-Oxazolone, 2-phenyl-4-(phenylmethylene)-
4-Benzyliden-2-phenyl-4,5-dihydro-1,3-oxazol-5-on
4-Benzylidene-2-phenyl-4,5-dihydro-1,3-oxazol-5-one
4-Benzylidene-2-phenyl-1,3-oxazol-5(4H)-one
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-SDNWHVSQSA-N

Formula: C16H11NO2

SMILES: O=C1OC(c2ccccc2)=NC1=Cc1ccccc1

Mol. weight [g/mol]: 249.26

CAS: 17606-70-1

Physical Properties

Property code	Value	Unit	Source
chs	-7778.10	kJ/mol	NIST Webbook
gf	326.78	kJ/mol	Joback Method
hf	103.92	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	73.04	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.031		Crippen Method
mcvol	186.740	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	798.04	K	Joback Method
tc	1083.82	K	Joback Method
tf	528.03	K	Joback Method
vc	0.704	m3/kmol	Joback 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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17606701&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.