4,5-Isoxazoledicarboxylic acid, 4,5-dihydro-3-phenyl-, dimethyl ester, cis-

Other names: 2-Isoxazoline-4,5-dicarboxylic acid, 3-phenyl-, dimethyl ester, cis-
Inchi: InChI=1S/C13H13NO5/c1-17-12(15)9-10(8-6-4-3-5-7-8)14-19-11(9)13(16)18-2/h3-7,9,11
InchiKey: RZUSIVILFUXVKH-KOLCDFICSA-N
Formula: C13H13NO5
SMILES: COC(=O)C1ON=C(c2ccccc2)C1C(=O)OC
Mol. weight [g/mol]: 263.25
CAS: 17669-30-6

Physical Properties

Property code	Value	Unit	Source
chs	-6109.00	kJ/mol	NIST Webbook
gf	-217.02	kJ/mol	Joback Method
hf	-539.30	kJ/mol	Joback Method
hfs	-864.80	kJ/mol	NIST Webbook
hfus	38.00	kJ/mol	Joback Method
hvap	76.74	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	0.752		Crippen Method
mcvol	185.840	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
tb	771.50	K	Joback Method
tc	1011.41	K	Joback Method
tf	525.06	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.79	J/mol×K	771.50	Joback Method
cpg	568.16	J/mol×K	811.49	Joback Method
cpg	581.10	J/mol×K	851.47	Joback Method
cpg	592.58	J/mol×K	891.46	Joback Method
cpg	602.59	J/mol×K	931.44	Joback Method
cpg	611.12	J/mol×K	971.43	Joback Method

cpg	618.15	J/mol×K	1011.41	Joback Method

Sources

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=C17669306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfs:	Solid phase 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