(4R,5S)-(+)-4-Methyl-5-phenyl-2-oxazolidinone

Other names: (4R,5S)-4-Methyl-5-phenyl-2-oxazolidinone
4-Methyl-5-phenyl-1,3-oxazolidin-2-one-, (4R-cis)-
2-Oxazolidinone, 4-methyl-5-phenyl-, (4R-cis)-
Inchi: InChI=1S/C10H11NO2/c1-7-9(13-10(12)11-7)8-5-3-2-4-6-8/h2-7,9H,1H3,(H,11,12)
InchiKey: PPIBJOQGAJBQDF-UHFFFAOYSA-N
Formula: C10H11NO2
SMILES: CC1NC(=O)OC1c1ccccc1
Mol. weight [g/mol]: 177.20
CAS: 77943-39-6

Physical Properties

Property code	Value	Unit	Source
gf	53.57	kJ/mol	Joback Method
hf	-204.95	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	55.59	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.856		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	608.81	K	Joback Method
tc	866.14	K	Joback Method
tf	435.36	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.01	J/mol×K	608.81	Joback Method
cpg	362.13	J/mol×K	651.70	Joback Method
cpg	378.06	J/mol×K	694.59	Joback Method
cpg	392.79	J/mol×K	737.48	Joback Method
cpg	406.31	J/mol×K	780.36	Joback Method
cpg	418.63	J/mol×K	823.25	Joback Method

cpg	429.73	J/mol×K	866.14	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=C77943396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume