

(S)-(+)-4-Isopropyl-2-oxazolidinone

Other names:	(4S)-4-Isopropyl-2-oxazolidinone (4S)-(-)-Isopropyl-2-oxazolidinone
Inchi:	InChI=1S/C6H11NO2/c1-4(2)5-3-9-6(8)7-5/h4-5H,3H2,1-2H3,(H,7,8)/t5-/m0/s1
InchiKey:	YBUPWRYTXGAWJX-YFKPBYRVSA-N
Formula:	C6H11NO2
SMILES:	CC(C)C1COC(O)=N1
Mol. weight [g/mol]:	129.16
CAS:	17016-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-52.08	kJ/mol	Joback Method
hf	-278.92	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	57.17	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.955		Crippen Method
mcvol	101.960	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
tb	528.49	K	Joback Method
tc	732.67	K	Joback Method
tf	325.49	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.34	J/molxK	528.49	Joback Method
cpg	268.44	J/molxK	562.52	Joback Method
cpg	279.93	J/molxK	596.55	Joback Method
cpg	290.81	J/molxK	630.58	Joback Method
cpg	301.09	J/molxK	664.61	Joback Method
cpg	310.78	J/molxK	698.64	Joback Method
cpg	319.87	J/molxK	732.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C17016830&Units=SI

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
h vap:	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

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