(4S)-(-)-4-Isopropyl-1,3-oxazolidine-2-thione

Inchi: InChI=1S/C6H11NOS/c1-4(2)5-3-8-6(9)7-5/h4-5H,3H2,1-2H3,(H,7,9)/t5-/m0/s1
InchiKey: CIRDXQWBLPPFPN-YFKPBYRVSA-N
Formula: C6H11NOS
SMILES: CC(C)C1COC(S)=N1
Mol. weight [g/mol]: 145.22
CAS: 84272-19-5

Physical Properties

Property code	Value	Unit	Source
gf	114.13	kJ/mol	Joback Method
hf	-88.21	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	47.23	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.327		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	499.17	K	Joback Method
tc	742.36	K	Joback Method
tf	301.13	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.15	J/mol×K	499.17	Joback Method
cpg	268.05	J/mol×K	539.70	Joback Method
cpg	282.08	J/mol×K	580.23	Joback Method
cpg	295.25	J/mol×K	620.77	Joback Method
cpg	307.57	J/mol×K	661.30	Joback Method
cpg	319.04	J/mol×K	701.83	Joback Method
cpg	329.67	J/mol×K	742.36	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=C84272195&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
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