(4R,5S)-(+)-4-Methyl-5-phenyl-1,3-oxazolidine-2-th

Inchi: InChI=1S/C10H11NOS/c1-7-9(12-10(13)11-7)8-5-3-2-4-6-8/h2-7,9H,1H3,(H,11,13)
InchiKey: KQSZLXCAZDPTNY-UHFFFAOYSA-N
Formula: C10H11NOS
SMILES: CC1N=C(S)OC1c1ccccc1
Mol. weight [g/mol]: 193.26
CAS: 91794-28-4

Physical Properties

Property code	Value	Unit	Source
gf	254.95	kJ/mol	Joback Method
hf	50.70	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.432		Crippen Method
mcvol	145.040	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	613.14	K	Joback Method
tc	885.79	K	Joback Method
tf	383.39	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.62	J/mol×K	613.14	Joback Method
cpg	384.27	J/mol×K	658.58	Joback Method
cpg	400.44	J/mol×K	704.02	Joback Method
cpg	415.17	J/mol×K	749.46	Joback Method
cpg	428.48	J/mol×K	794.91	Joback Method
cpg	440.40	J/mol×K	840.35	Joback Method
cpg	450.99	J/mol×K	885.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91794284&Units=SI
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

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