S-(+)-S-Methyl-S-phenylsulfoxime

Inchi: InChI=1S/C7H9NOS/c1-10(8,9)7-5-3-2-4-6-7/h2-6,8H,1H3/t10-/m1/s1
InchiKey: YFYIDTVGWCYSEO-SNVBAGLBSA-N
Formula: C7H9NOS
SMILES: CS(=N)(=O)c1ccccc1
Mol. weight [g/mol]: 155.22
CAS: 33903-50-3

Physical Properties

Property code	Value	Unit	Source
gf	22.42	kJ/mol	Joback Method
hf	-63.32	kJ/mol	Joback Method
hvap	58.35	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.722		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
tb	527.60	K	Joback Method
tf	300.46	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.10	J/mol×K	527.60	Joback Method
cpg	52.67	J/mol×K	100.12	Joback Method
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cpg	52.67	J/mol×K	100.12	Joback Method
cpg	52.67	J/mol×K	100.12	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=C33903503&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point