R-(-)-N,S-Dimethyl-S-phenylsulfoximine

Inchi: InChI=1S/C8H11NOS/c1-9-11(2,10)8-6-4-3-5-7-8/h3-7H,1-2H3/t11-/m0/s1
InchiKey: OQWUXWSLVBGOIX-NSHDSACASA-N
Formula: C8H11NOS
SMILES: CN=S(C)(=O)c1ccccc1
Mol. weight [g/mol]: 169.24
CAS: 20414-85-1

Physical Properties

Property code	Value	Unit	Source
hf	-209.86	kJ/mol	Joback Method
hvap	51.89	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.773		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	542.70	K	Joback Method
tc	779.53	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20414851&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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