S-(-)-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-LLVKDONJSA-N
Formula: C8H11NOS
SMILES: CN=[S@@](C)(=O)c1ccccc1
Mol. weight [g/mol]: 169.25

Physical Properties

Property code	Value	Unit	Source
hf	-79.91	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-1.25		Cheméo Relay (1.0)
logp	1.773		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
tb	557.51	K	Cheméo Relay (1.0)
tf	349.19	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33993532&Units=SI
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
ie: Ionization energy
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