.alpha.-Methylthio-.beta.-(4-nitrophenyl)thiostyren
(E)

InChI: InChI=1S/C15H13NO2S2/c1-19-15(12-5-3-2-4-6-12)11-20-14-9-7-13(8-10-14)16(17)18/h
InChIKey: MKYPVELDKWUVSU-PTNGSMBKSA-N
Formula: C15H13NO2S2
SMILES: CS/C(=C/Sc1ccc([N+](=O)[O-])cc1)c1ccccc1
Mol. weight [g/mol]: 303.41

Physical Properties

Property code	Value	Unit	Source
hf	244.33	kJ/mol	Cheméo Relay (1.0)
hfus	40.81	kJ/mol	Joback Method
hvap	114.14	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
log10ws	-5.69		Cheméo Relay (1.0)
logp	5.048		Crippen Method
mcvol	220.510	ml/mol	McGowan Method
tb	674.60	K	Cheméo Relay (1.0)
tf	382.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.73	J/mol×K	894.38	Joback Method
cpg	609.81	J/mol×K	944.22	Joback Method
cpg	620.48	J/mol×K	994.07	Joback Method
cpg	629.88	J/mol×K	1043.91	Joback Method
cpg	638.18	J/mol×K	1093.75	Joback Method
cpg	645.53	J/mol×K	1143.60	Joback Method
cpg	652.07	J/mol×K	1193.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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?Str2File=C29624279
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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