METHYL N'-TOSYLCARBAMIMIDOTHIOATE

Other names: Isothiourea, 2-methyl-3-(4-methylphenylsulfonyl)-
S-methyl-N'-tosylisothiourea
Inchi: InChI=1S/C9H12N2O2S2/c1-7-3-5-8(6-4-7)15(12,13)11-9(10)14-2/h3-6H,1-2H3,(H2,10,1
InchiKey: ZWAMEGGTEJHAOT-UHFFFAOYSA-N
Formula: C9H12N2O2S2
SMILES: CS/C(N)=N/S(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 244.34

Physical Properties

Property code	Value	Unit	Source
hf	-218.93	kJ/mol	Cheméo Relay (1.0)
hvap	92.39	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-3.31		Cheméo Relay (1.0)
logp	1.361		Crippen Method
mcvol	174.010	ml/mol	McGowan Method
tf	405.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.20	kJ/mol	401.20	NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2651163&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point