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:	CSC(N)=NS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	244.33
CAS:	2651-16-3

Physical Properties

Property code	Value	Unit	Source
hf	-309.29	kJ/mol	Joback Method
hvap	78.05	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.361		Crippen Method
mcvol	174.010	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	702.63	K	Joback Method
tc	950.83	K	Joback Method

Temperature Dependent Properties

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

Sources

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=C2651163&Units=SI
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
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