Benzenamine, 4-isothiocyanato-N,N-dimethyl-

Other names:	p-(Dimethylamino)phenyl isothiocyanate
	p-(N,N-Dimethylamino)phenyl isothiocyanate
	Isothiocyanic acid, p-(dimethylamino)phenyl ester
	TL 1106
	4-(Dimethylamino)phenyl isothiocyanate
	4-(N,N-Dimethylamino)phenyl isothiocyanate
	4-Isothiocyanato-N,N-dimethylaniline
	Phenylisothiocyanate, 4-dimethylamino
	NSC 196179
Inchi:	InChI=1S/C9H10N2S/c1-11(2)9-5-3-8(4-6-9)10-7-12/h3-6H,1-2H3
InchiKey:	HRDJPEMAGYHSJR-UHFFFAOYSA-N
Formula:	C9H10N2S
SMILES:	CN(C)c1ccc(N=C=S)cc1
Mol. weight [g/mol]:	178.25
CAS:	2131-64-8

Physical Properties

Property code	Value	Unit	Source
hf	347.57	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.487		Crippen Method
mcvol	141.620	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	595.37	K	Joback Method
tc	845.80	K	Joback Method

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=C2131648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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