Trityl isothiocyanate

Other names: Triphenylmethyl isothiocyanate
Inchi: InChI=1S/C20H15NS/c22-16-21-20(17-10-4-1-5-11-17,18-12-6-2-7-13-18)19-14-8-3-9-15
InchiKey: ZPZHAUXTGFNYTN-UHFFFAOYSA-N
Formula: C20H15NS
SMILES: S=C=NC(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 301.40
CAS: 1726-94-9

Physical Properties

Property code	Value	Unit	Source
hf	528.78	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.081		Crippen Method
mcvol	239.110	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
tb	879.76	K	Joback Method
tc	1182.54	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C1726949&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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