4,4'-Methylenebis(3-chlorophenyl)diisothiocyanat

Inchi: InChI=1S/C15H8Cl2N2S2/c16-12-6-10(1-3-14(12)18-8-20)5-11-2-4-15(19-9-21)13(17)7-
InchiKey: GDOSNEJTWBTBOC-UHFFFAOYSA-N
Formula: C15H8Cl2N2S2
SMILES: S=C=Nc1ccc(Cc2ccc(N=C=S)c(Cl)c2)cc1Cl
Mol. weight [g/mol]: 351.27
CAS: 210101-80-7

Physical Properties

Property code	Value	Unit	Source
hf	610.91	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.053		Crippen Method
mcvol	234.630	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
tb	982.64	K	Joback Method
tc	1284.49	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C210101807&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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