

Ethyl 3-Chloro-4-methylthiolcarbanilate

Inchi:	InChI=1S/C10H12ClNOS/c1-3-14-10(13)12-8-5-4-7(2)9(11)6-8/h4-6H,3H2,1-2H3,(H,12,13)
InchiKey:	PCXVSKLBAGHKHW-UHFFFAOYSA-N
Formula:	C10H12ClNOS
SMILES:	CCSC(O)=Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]:	229.73
CAS:	209683-36-3

Physical Properties

Property code	Value	Unit	Source
hf	-89.81	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.947		Crippen Method
mcvol	168.140	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	739.79	K	Joback Method
tc	970.91	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=C209683363&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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