Benzene, 1-chloro-4-(isothiocyanatomethyl)-

Other names:	Isothiocyanic acid, p-chlorobenzyl ester
	4-Chlorobenzyl isothiocyanate
Inchi:	InChI=1S/C8H6ClNS/c9-8-3-1-7(2-4-8)5-10-6-11/h1-4H,5H2
InchiKey:	DEHXIHUIYSXZNH-UHFFFAOYSA-N
Formula:	C8H6ClNS
SMILES:	S=C=NCc1ccc(Cl)cc1
Mol. weight [g/mol]:	183.66
CAS:	3694-45-9

Physical Properties

Property code	Value	Unit	Source
hf	284.94	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.943		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	597.48	K	Joback Method
tc	862.02	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3694459&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