

Isothiocyanic acid, m-chlorobenzyl ester

Other names:	Benzene, 1-chloro-3-(isothiocyanatomethyl)- m-Chlorobenzyl isothiocyanate 3-Chlorobenzyl isothiocyanate Isothiocyanic acid, 3-chlorobenzyl ester
Inchi:	InChI=1S/C8H6ClNS/c9-8-3-1-2-7(4-8)5-10-6-11/h1-4H,5H2
InchiKey:	GGNLZOLEJMSOKU-UHFFFAOYSA-N
Formula:	C8H6ClNS
SMILES:	<chem>S=C=NCc1cccc(Cl)c1</chem>
Mol. weight [g/mol]:	183.66
CAS:	3694-58-4

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3694584&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

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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