

4-Chlorophenyl isothiocyanate

Other names:	p-Chlorophenyl isothiocyanate Benzene, 1-chloro-4-isothiocyanato- Isothiocyanic acid, p-chlorophenyl ester Isothiocyanic acid, 4-chlorophenyl ester 1-Chloro-4-isothiocyanatobenzene 4-Chlor-phenyl-isothiocyanat
Inchi:	InChI=1S/C7H4CINS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H
InchiKey:	MZZVFXMTZTVUFO-UHFFFAOYSA-N
Formula:	C7H4CINS
SMILES:	S=C=Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	169.63
CAS:	2131-55-7

Physical Properties

Property code	Value	Unit	Source
hf	305.58	kJ/mol	Joback Method
hvap	48.94	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	3.074		Crippen Method
mcvol	115.700	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	574.60	K	Joback Method
tc	845.67	K	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.00 ± 1.00	K	2.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

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