

4-Chlorobenzyl isothiocyanate

Other names:	Isothiocyanic acid, p-chlorobenzyl ester 4-Chlorobenzyl isothiocyanate
Inchi:	InChI=1S/C8H6CINS/c9-8-3-1-7(2-4-8)5-10-6-11/h1-4H,5H2
InchiKey:	DEHXIHUIYSXZNH-UHFFFAOYSA-N
Formula:	C8H6CINS
SMILES:	S=C=NCc1ccc(Cl)cc1
Mol. weight [g/mol]:	183.66

Physical Properties

Property code	Value	Unit	Source
ie	8.48	eV	Cheméo Relay (1.0)
logp	2.943		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
tb	524.51	K	Cheméo Relay (1.0)
tf	315.71	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3694459&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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