2-Chlorobenzyl isothiocyanate

Other names:	Isothiocyanic acid, o-chlorobenzyl ester
	2-Chlorobenzyl isothiocyanate
Inchi:	InChI=1S/C8H6ClNS/c9-8-4-2-1-3-7(8)5-10-6-11/h1-4H,5H2
InchiKey:	RMVDNJDSLXQPAV-UHFFFAOYSA-N
Formula:	C8H6ClNS
SMILES:	S=C=NCc1ccccc1Cl
Mol. weight [g/mol]:	183.66

Physical Properties

Property code	Value	Unit	Source
logp	2.943		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
tb	523.90	K	Cheméo Relay (1.0)
tf	299.67	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C18967447&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point