4-Chlorobenzyl isothiocyanate

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

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/ci990307l

Legend

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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point