

3-Chlorobenzoyl isothiocyanate

Inchi: InChI=1S/C8H4ClNOS/c9-7-3-1-2-6(4-7)8(11)10-5-12/h1-4H
InchiKey: ZUISLKTWVWIULT-UHFFFAOYSA-N
Formula: C8H4ClNOS
SMILES: O=C(N=C=S)c1cccc(Cl)c1
Mol. weight [g/mol]: 197.64
CAS: 66090-36-6

Physical Properties

Property code	Value	Unit	Source
hf	172.36	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.583		Crippen Method
mcpvol	131.360	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	651.35	K	Joback Method
tc	922.35	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C66090366&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

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
tc:	Critical Temperature

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