

Benzoic acid, 3-isothiocyanato-

Inchi:	InChI=1S/C8H5NO2S/c10-8(11)6-2-1-3-7(4-6)9-5-12/h1-4H,(H,10,11)
InchiKey:	PJRBPKOOGKLPFB-UHFFFAOYSA-N
Formula:	C8H5NO2S
SMILES:	O=C(O)c1cccc(N=C=S)c1
Mol. weight [g/mol]:	179.20
CAS:	2131-63-7

Physical Properties

Property code	Value	Unit	Source
hf	35.87	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.119		Crippen Method
mcvol	124.990	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	706.10	K	Joback Method
tc	948.49	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tc:	Critical Temperature

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