

4-Fluorobenzyl isothiocyanate

Other names:	Benzene, 1-fluoro-4-(isothiocyanatomethyl)-p-fluorobenzyl isothiocyanate
Inchi:	InChI=1S/C8H6FNS/c9-8-3-1-7(2-4-8)5-10-6-11/h1-4H,5H2
InchiKey:	LPVNPJMEWWUFHD-UHFFFAOYSA-N
Formula:	C8H6FNS
SMILES:	Fc1ccc(CN=C=S)cc1
Mol. weight [g/mol]:	167.20
CAS:	2740-88-7

Physical Properties

Property code	Value	Unit	Source
hf	104.57	kJ/mol	Joback Method
hvap	45.96	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.429		Crippen Method
mcvol	119.320	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	559.32	K	Joback Method
tc	806.48	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2740887&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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