

2-Fluorobenzyl isothiocyanate

Inchi: InChI=1S/C8H6FNS/c9-8-4-2-1-3-7(8)5-10-6-11/h1-4H,5H2
InchiKey: HHJNPMOABDDXEL-UHFFFAOYSA-N
Formula: C8H6FNS
SMILES: Fc1ccccc1CN=C=S
Mol. weight [g/mol]: 167.20
CAS: 64382-80-5

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: 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=C64382805&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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