

3-Fluorophenyl isocyanate

Other names:	m-Fluorophenyl isocyanate Benzene, 1-fluoro-3-isocyanato-4-fluorophenyl isocyanate
Inchi:	InChI=1S/C7H4FNO/c8-6-2-1-3-7(4-6)9-5-10/h1-4H
InchiKey:	RIKWVZGZRYDACA-UHFFFAOYSA-N
Formula:	C7H4FNO
SMILES:	O=C=Nc1cccc(F)c1
Mol. weight [g/mol]:	137.11
CAS:	404-71-7

Physical Properties

Property code	Value	Unit	Source
hf	-164.27	kJ/mol	Joback Method
hvap	42.83	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	1.793		Crippen Method
mcvol	94.750	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	457.16	K	Joback Method
tc	670.64	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=C404717&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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