3-FLUOROPHENYL ISOCYANATE

Other names: 4-fluorophenyl isocyanate
Benzene, 1-fluoro-3-isocyanato-
m-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

Physical Properties

Property code	Value	Unit	Source
hf	-176.69	kJ/mol	Cheméo Relay (1.0)
hvap	45.74	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-2.11		Cheméo Relay (1.0)
logp	1.793		Crippen Method
mcvol	94.750	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	422.08	K	Cheméo Relay (1.0)
tc	667.49	K	Cheméo Relay (1.0)

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C404717&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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