2-FLUOROPHENYL ISOCYANATE

Other names: Benzene, 1-fluoro-2-isocyanato-
Isocyanic acid o-fluorophenyl ester
o-Fluorophenyl isocyanate
Inchi: InChI=1S/C7H4FNO/c8-6-3-1-2-4-7(6)9-5-10/h1-4H
InchiKey: VZNCSZQPNIEEMN-UHFFFAOYSA-N
Formula: C7H4FNO
SMILES: O=C=Nc1ccccc1F
Mol. weight [g/mol]: 137.11

Physical Properties

Property code	Value	Unit	Source
hf	-159.18	kJ/mol	Cheméo Relay (1.0)
hvap	46.45	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
logp	1.793		Crippen Method
mcvol	94.750	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	400.50	K	Cheméo Relay (1.0)
tc	668.14	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16744982&Units=SI
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):

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature