

Urea, 3-(p-fluorophenyl)-1-methyl-1-nitroso-

Inchi:	InChI=1S/C8H8FN3O2/c1-12(11-14)8(13)10-7-4-2-6(9)3-5-7/h2-5H,1H3,(H,10,13)
InchiKey:	UBHNEXDJFIFPFN-UHFFFAOYSA-N
Formula:	C8H8FN3O2
SMILES:	CN(N=O)C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]:	197.17
CAS:	777-59-3

Physical Properties

Property code	Value	Unit	Source
hf	-339.27	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.971		Crippen Method
mcvol	134.670	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	593.25	K	Joback Method
tc	798.47	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C777593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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