

4-Ethoxyisonitrosoacetanilide

Inchi:	InChI=1S/C10H12N2O3/c1-2-15-9-5-3-8(4-6-9)12-10(13)7-11-14/h3-7,14H,2H2,1H3,(H,1)
InchiKey:	LCSKYCHMODBOPE-YRNVUSSQSA-N
Formula:	C10H12N2O3
SMILES:	CCOc1ccc(NC(=O)C=NO)cc1
Mol. weight [g/mol]:	208.21
CAS:	17122-74-6

Physical Properties

Property code	Value	Unit	Source
hf	-286.01	kJ/mol	Joback Method
hvap	76.38	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	1.484		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	755.18	K	Joback Method
tc	967.92	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	7.60	kJ/mol	490.00	NIST Webbook
hfust	7.60	kJ/mol	491.20	NIST Webbook
hfust	7.60	kJ/mol	490.00	NIST Webbook
sfust	15.50	J/molxK	490.00	NIST Webbook

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=C17122746&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvp:	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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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