2-Methoxyisonitrosoacetanilide

Inchi: InChI=1S/C9H10N2O3/c1-14-8-5-3-2-4-7(8)11-9(12)6-10-13/h2-6,13H,1H3,(H,11,12)/b10
InchiKey: XJTPRORZFBOGBA-UXBLZVDNSA-N
Formula: C9H10N2O3
SMILES: COc1ccccc1NC(=O)C=NO
Mol. weight [g/mol]: 194.19
CAS: 6335-42-8

Physical Properties

Property code	Value	Unit	Source
hf	-265.37	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	1.094		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	732.30	K	Joback Method
tc	947.81	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.80	kJ/mol	424.60	NIST Webbook
hfust	27.80	kJ/mol	422.00	NIST Webbook
sfust	65.90	J/mol×K	422.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6335428&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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