2-Chloroisonitrosoacetanilide

Inchi: InChI=1S/C8H7ClN2O2/c9-6-3-1-2-4-7(6)11-8(12)5-10-13/h1-5,13H,(H,11,12)/b10-5+
InchiKey: VFTUFVGOXLZZPW-BJMVGYQFSA-N
Formula: C8H7ClN2O2
SMILES: O=C(C=NO)Nc1ccccc1Cl
Mol. weight [g/mol]: 198.61
CAS: 14722-82-8

Physical Properties

Property code	Value	Unit	Source
hf	-128.25	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.738		Crippen Method
mcvol	135.160	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	724.43	K	Joback Method
tc	948.67	K	Joback Method
tf	429.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.70	kJ/mol	432.70	NIST Webbook
hfust	29.70	kJ/mol	429.00	NIST Webbook
sfust	69.30	J/mol×K	429.00	NIST Webbook

Sources

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=C14722828&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tf:	Normal melting (fusion) point