Carbanilide, n-nitroso-

Inchi: InChI=1S/C13H11N3O2/c17-13(14-11-7-3-1-4-8-11)16(15-18)12-9-5-2-6-10-12/h1-10H,(
InchiKey: OCRGVJSSFMUOIH-UHFFFAOYSA-N
Formula: C13H11N3O2
SMILES: O=NN(C(=O)Nc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 241.25
CAS: 60285-31-6

Physical Properties

Property code	Value	Unit	Source
hf	1.64	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.406		Crippen Method
mcvol	179.590	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	730.08	K	Joback Method
tc	966.42	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60285316&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
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