1-(2-Chloro-3-(1-[(cyclohexylamino)carbonyl]-2-ox

Inchi: InChI=1S/C17H29ClN6O4/c18-13(11-23(21-27)16(25)19-14-7-3-1-4-8-14)12-24(22-28)17

InchiKey: LOCWSNJMMKPGFO-UHFFFAOYSA-N

Formula: C17H29ClN6O4

SMILES: O=NN(CC(Cl)CN(N=O)C(=O)NC1CCCCC1)C(=O)NC1CCCCC1

Mol. weight [g/mol]: 416.90

CAS: 33024-51-0

Physical Properties

Property code	Value	Unit	Source
hf	-626.13	kJ/mol	Joback Method
hvap	106.93	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	3.645		Crippen Method
mcvol	307.070	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
tb	1024.21	K	Joback Method
tc	1257.04	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33024510&Units=SI

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