Carbamic acid, n-methyl, n-nitroso-, 4[2-(n'-methyl-n'-nitroso-ureido)ethyl]phenyl ester

Inchi: InChI=1S/C12H15N5O5/c1-16(14-20)11(18)13-8-7-9-3-5-10(6-4-9)22-12(19)17(2)15-21/h
InchiKey: LBYHODFAESFBFB-UHFFFAOYSA-N
Formula: C12H15N5O5
SMILES: CN(N=O)C(=O)NCCc1ccc(OC(=O)N(C)N=O)cc1
Mol. weight [g/mol]: 309.28
CAS: 61295-75-8

Physical Properties

Property code	Value	Unit	Source
hf	-571.18	kJ/mol	Joback Method
hvap	89.86	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	1.664		Crippen Method
mcvol	218.230	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	837.63	K	Joback Method
tc	1043.71	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61295758&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