Urea, 1-(2-chloroethyl)-1-nitroso-3-(p-tolylsulfonyl)-

Inchi: InChI=1S/C10H12ClN3O4S/c1-8-2-4-9(5-3-8)19(17,18)12-10(15)14(13-16)7-6-11/h2-5H,

InchiKey: OJNXBFXPODIQKI-UHFFFAOYSA-N

Formula: C10H12ClN3O4S

SMILES: Cc1ccc(S(=O)(=O)NC(=O)N(CCCl)N=O)cc1

Mol. weight [g/mol]: 305.74

CAS: 33024-34-9

Physical Properties

Property code	Value	Unit	Source
hf	-653.53	kJ/mol	Joback Method
hvap	88.13	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	1.616		Crippen Method
mcvol	201.410	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	724.95	K	Joback Method
tc	930.41	K	Joback Method

Sources

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=C33024349&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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