

Urea, 1-(2-chloroethyl)-3-[p-(dimethylcarbamoyl)phenyl]

Inchi:	InChI=1S/C12H15ClN4O3/c1-16(2)11(18)9-3-5-10(6-4-9)14-12(19)17(15-20)8-7-13/h3-6
InchiKey:	PZDRJSZTIYNYJZ-UHFFFAOYSA-N
Formula:	C12H15ClN4O3
SMILES:	CN(C)C(=O)c1ccc(NC(=O)N(CCCl)N=O)cc1
Mol. weight [g/mol]:	298.73
CAS:	13909-28-9

Physical Properties

Property code	Value	Unit	Source
hf	-286.51	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.143		Crippen Method
mcvol	213.050	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	789.24	K	Joback Method
tc	999.78	K	Joback Method

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=C13909289&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
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

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