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

Inchi: InChI=1S/C12H16ClN3O2/c1-16(2)11(17)9-3-5-10(6-4-9)15-12(18)14-8-7-13/h3-6H,7-8H

InchiKey: ZGLCEZMUTDVHOD-UHFFFAOYSA-N

Formula: C12H16ClN3O2

SMILES: CN(C)C(=O)c1ccc(NC(=O)NCCCl)cc1

Mol. weight [g/mol]: 269.73

CAS: 13908-49-1

Physical Properties

Property code	Value	Unit	Source
gf	172.73	kJ/mol	Joback Method
hf	-132.38	kJ/mol	Joback Method
hfus	41.10	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.749		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	763.57	K	Joback Method
tc	979.35	K	Joback Method
tf	531.51	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.57	J/mol×K	763.57	Joback Method
cpg	562.68	J/mol×K	799.53	Joback Method
cpg	573.88	J/mol×K	835.50	Joback Method
cpg	584.22	J/mol×K	871.46	Joback Method
cpg	593.76	J/mol×K	907.42	Joback Method
cpg	602.55	J/mol×K	943.38	Joback Method
cpg	610.63	J/mol×K	979.35	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=C13908491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume