Urea, 1-(2-chloroethyl)-3-(p-methoxyphenyl)-

Inchi: InChI=1S/C10H13ClN2O2/c1-15-9-4-2-8(3-5-9)13-10(14)12-7-6-11/h2-5H,6-7H2,1H3,(H
InchiKey: CNYYWOOAIIXDLZ-UHFFFAOYSA-N
Formula: C10H13ClN2O2
SMILES: COc1ccc(NC(=O)NCCCl)cc1
Mol. weight [g/mol]: 228.68
CAS: 65536-40-5

Physical Properties

Property code	Value	Unit	Source
gf	69.03	kJ/mol	Joback Method
hf	-178.27	kJ/mol	Joback Method
hfus	32.49	kJ/mol	Joback Method
hvap	67.20	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.055		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	673.92	K	Joback Method
tc	890.45	K	Joback Method
tf	448.80	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.21	J/mol×K	673.92	Joback Method
cpg	433.37	J/mol×K	710.01	Joback Method
cpg	444.72	J/mol×K	746.10	Joback Method
cpg	455.27	J/mol×K	782.19	Joback Method
cpg	465.04	J/mol×K	818.27	Joback Method
cpg	474.06	J/mol×K	854.36	Joback Method
cpg	482.35	J/mol×K	890.45	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=C65536405&Units=SI

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