Urea, 1-(4-acetylphenyl)-3-(2-chloroethyl)-

Inchi: InChI=1S/C11H13ClN2O2/c1-8(15)9-2-4-10(5-3-9)14-11(16)13-7-6-12/h2-5H,6-7H2,1H3
InchiKey: XKYQSDGJEOAYOC-UHFFFAOYSA-N
Formula: C11H13ClN2O2
SMILES: CC(=O)c1ccc(NC(=O)NCCCl)cc1
Mol. weight [g/mol]: 240.69
CAS: 13908-48-0

Physical Properties

Property code	Value	Unit	Source
gf	53.53	kJ/mol	Joback Method
hf	-179.27	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.249		Crippen Method
mcvol	177.430	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
tb	728.25	K	Joback Method
tc	949.77	K	Joback Method
tf	487.77	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.44	J/mol×K	728.25	Joback Method
cpg	470.91	J/mol×K	765.17	Joback Method
cpg	481.51	J/mol×K	802.09	Joback Method
cpg	491.29	J/mol×K	839.01	Joback Method
cpg	500.29	J/mol×K	875.93	Joback Method
cpg	508.55	J/mol×K	912.85	Joback Method
cpg	516.12	J/mol×K	949.77	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=C13908480&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