1-(4-chlorophenyl)-1,3-dimethylurea

Other names: Urea, N-(4-chlorophenyl)-N,N'-dimethyl-
Inchi: InChI=1S/C9H11ClN2O/c1-11-9(13)12(2)8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)
InchiKey: XZTUYISAOWDOSC-UHFFFAOYSA-N
Formula: C9H11ClN2O
SMILES: CNC(=O)N(C)c1ccc(Cl)cc1
Mol. weight [g/mol]: 198.65
CAS: 13578-25-1

Physical Properties

Property code	Value	Unit	Source
gf	187.00	kJ/mol	Joback Method
hf	-11.35	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.116		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	590.89	K	Joback Method
tc	811.66	K	Joback Method
tf	395.11	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.65	J/mol×K	590.89	Joback Method
cpg	350.07	J/mol×K	627.68	Joback Method
cpg	361.63	J/mol×K	664.48	Joback Method
cpg	372.36	J/mol×K	701.27	Joback Method
cpg	382.31	J/mol×K	738.07	Joback Method
cpg	391.52	J/mol×K	774.86	Joback Method
cpg	400.03	J/mol×K	811.66	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=C13578251&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