1-(M-chlorophenyl)biuret

Inchi: InChI=1S/C8H8ClN3O2/c9-5-2-1-3-6(4-5)11-8(14)12-7(10)13/h1-4H,(H4,10,11,12,13,14)
InchiKey: BDGYTVITCGVFQP-UHFFFAOYSA-N
Formula: C8H8ClN3O2
SMILES: NC(=O)NC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 213.62
CAS: 116346-10-2

Physical Properties

Property code	Value	Unit	Source
gf	94.72	kJ/mol	Joback Method
hf	-83.56	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	77.73	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	1.540		Crippen Method
mcvol	145.140	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	732.14	K	Joback Method
tc	971.45	K	Joback Method
tf	537.22	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.08	J/mol×K	732.14	Joback Method
cpg	369.94	J/mol×K	772.03	Joback Method
cpg	378.01	J/mol×K	811.91	Joback Method
cpg	385.32	J/mol×K	851.80	Joback Method
cpg	391.91	J/mol×K	891.68	Joback Method
cpg	397.84	J/mol×K	931.57	Joback Method
cpg	403.13	J/mol×K	971.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346102&Units=SI
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

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