N,N'-(4-Chloro-O-phenylene)bisacetamide

Other names: N-(2-Acetamido-5-chloro-phenyl)acetamide
Inchi: InChI=1S/C10H11ClN2O2/c1-6(14)12-9-4-3-8(11)5-10(9)13-7(2)15/h3-5H,1-2H3,(H,12,1
InchiKey: VDFQABAPEFACAU-UHFFFAOYSA-N
Formula: C10H11ClN2O2
SMILES: CC(=O)Nc1ccc(Cl)cc1NC(C)=O
Mol. weight [g/mol]: 226.66
CAS: 86569-36-0

Physical Properties

Property code	Value	Unit	Source
gf	35.48	kJ/mol	Joback Method
hf	-170.10	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.257		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	2132.00		NIST Webbook
tb	710.35	K	Joback Method
tc	936.42	K	Joback Method
tf	489.02	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.13	J/mol×K	710.35	Joback Method
cpg	417.89	J/mol×K	748.03	Joback Method
cpg	427.86	J/mol×K	785.71	Joback Method
cpg	437.05	J/mol×K	823.38	Joback Method
cpg	445.50	J/mol×K	861.06	Joback Method
cpg	453.23	J/mol×K	898.74	Joback Method
cpg	460.28	J/mol×K	936.42	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=C86569360&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume