N-(2-Acetamido-4-chlorophenyl)-N-acetylacetamid

Other names: N-(2-Acetamido-5-chlorophenyl)diacetamide
Inchi: InChI=1S/C12H13ClN2O3/c1-7(16)14-11-6-10(13)4-5-12(11)15(8(2)17)9(3)18/h4-6H,1-3
InchiKey: AJOVFKRJVSDKSU-UHFFFAOYSA-N
Formula: C12H13ClN2O3
SMILES: CC(=O)Nc1cc(Cl)ccc1N(C(C)=O)C(C)=O
Mol. weight [g/mol]: 268.70

Physical Properties

Property code	Value	Unit	Source
gf	-55.21	kJ/mol	Joback Method
hf	-309.90	kJ/mol	Joback Method
hfus	37.21	kJ/mol	Joback Method
hvap	79.01	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.198		Crippen Method
mcvol	193.090	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
tb	772.25	K	Joback Method
tc	995.06	K	Joback Method
tf	541.30	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.69	J/mol×K	772.25	Joback Method
cpg	520.66	J/mol×K	809.39	Joback Method
cpg	530.76	J/mol×K	846.52	Joback Method
cpg	540.01	J/mol×K	883.66	Joback Method
cpg	548.47	J/mol×K	920.79	Joback Method
cpg	556.18	J/mol×K	957.93	Joback Method
cpg	563.18	J/mol×K	995.06	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=U373411&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume