Ethanediamine, N-acetyl-N'-(4-chlorophenoxyacetyl)

Inchi: InChI=1S/C12H15ClN2O3/c1-9(16)14-6-7-15-12(17)8-18-11-4-2-10(13)3-5-11/h2-5H,6-8

InchiKey: TWXOVAKWKRNSFO-UHFFFAOYSA-N

Formula: C12H15ClN2O3

SMILES: CC(=O)NCCNC(=O)COc1ccc(Cl)cc1

Mol. weight [g/mol]: 270.71

Physical Properties

Property code	Value	Unit	Source
gf	-43.05	kJ/mol	Joback Method
hf	-332.13	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	0.971		Crippen Method
mcvol	197.390	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	773.55	K	Joback Method
tc	989.88	K	Joback Method
tf	521.27	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.59	J/mol×K	773.55	Joback Method
cpg	548.23	J/mol×K	809.60	Joback Method
cpg	558.98	J/mol×K	845.66	Joback Method
cpg	568.86	J/mol×K	881.71	Joback Method
cpg	577.89	J/mol×K	917.77	Joback Method
cpg	586.09	J/mol×K	953.82	Joback Method
cpg	593.50	J/mol×K	989.88	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=R408881&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