Ethanediamine, N-(4-methoxyphenyl)-N,N'-diacetyl

Inchi: InChI=1S/C13H18N2O3/c1-10(16)15(11(2)17)9-8-14-12-4-6-13(18-3)7-5-12/h4-7,14H,8-9

InchiKey: CBTZQWVXGNIEMO-UHFFFAOYSA-N

Formula: C13H18N2O3

SMILES: COc1ccc(NCCN(C(C)=O)C(C)=O)cc1

Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-1.31	kJ/mol	Joback Method
hf	-322.97	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.502		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	721.27	K	Joback Method
tc	929.37	K	Joback Method
tf	482.43	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.02	J/mol×K	721.27	Joback Method
cpg	566.92	J/mol×K	755.95	Joback Method
cpg	579.89	J/mol×K	790.64	Joback Method
cpg	591.94	J/mol×K	825.32	Joback Method
cpg	603.12	J/mol×K	860.00	Joback Method
cpg	613.44	J/mol×K	894.69	Joback Method
cpg	622.95	J/mol×K	929.37	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=R404423&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