Ethanediamine, N-(1,3-benzodioxol-5-ylmethyl), N,N'-diacetyl

Inchi: InChI=1S/C14H18N2O4/c1-10(17)15-5-6-16(11(2)18)8-12-3-4-13-14(7-12)20-9-19-13/h3

InchiKey: VBUZYSAZBMAJEG-UHFFFAOYSA-N

Formula: C14H18N2O4

SMILES: CC(=O)NCCN(Cc1ccc2c(c1)OCO2)C(C)=O

Mol. weight [g/mol]: 278.30

Physical Properties

Property code	Value	Unit	Source
gf	-1.30	kJ/mol	Joback Method
hf	-393.72	kJ/mol	Joback Method
hfus	49.62	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	0.900		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	792.02	K	Joback Method
tc	1008.83	K	Joback Method
tf	559.31	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.97	J/mol×K	792.02	Joback Method
cpg	631.77	J/mol×K	828.16	Joback Method
cpg	643.71	J/mol×K	864.29	Joback Method
cpg	654.85	J/mol×K	900.43	Joback Method
cpg	665.27	J/mol×K	936.56	Joback Method
cpg	675.06	J/mol×K	972.70	Joback Method
cpg	684.28	J/mol×K	1008.83	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=R408821&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