4-Amino-1-butanol, N,O-diacetyl-

Inchi: InChI=1S/C8H15NO3/c1-7(10)9-5-3-4-6-12-8(2)11/h3-6H2,1-2H3,(H,9,10)
InchiKey: KZIDOIUZBLXFCT-UHFFFAOYSA-N
Formula: C8H15NO3
SMILES: CC(=O)NCCCCOC(C)=O
Mol. weight [g/mol]: 173.21

Physical Properties

Property code	Value	Unit	Source
gf	-256.97	kJ/mol	Joback Method
hf	-512.36	kJ/mol	Joback Method
hfus	25.96	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.466		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1482.00		NIST Webbook
tb	562.77	K	Joback Method
tc	749.30	K	Joback Method
tf	354.67	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.46	J/mol×K	562.77	Joback Method
cpg	357.34	J/mol×K	593.86	Joback Method
cpg	368.69	J/mol×K	624.95	Joback Method
cpg	379.52	J/mol×K	656.03	Joback Method
cpg	389.82	J/mol×K	687.12	Joback Method
cpg	399.62	J/mol×K	718.21	Joback Method
cpg	408.90	J/mol×K	749.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352302&Units=SI
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

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