5-Amino-1-pentanol, N,O-diacetyl-

Inchi: InChI=1S/C9H17NO3/c1-8(11)10-6-4-3-5-7-13-9(2)12/h3-7H2,1-2H3,(H,10,11)
InchiKey: KTZISYASHVHEIR-UHFFFAOYSA-N
Formula: C9H17NO3
SMILES: CC(=O)NCCCCCOC(C)=O
Mol. weight [g/mol]: 187.24

Physical Properties

Property code	Value	Unit	Source
gf	-248.55	kJ/mol	Joback Method
hf	-533.00	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	57.97	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	0.856		Crippen Method
mcvol	156.660	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1589.50		NIST Webbook
tb	585.65	K	Joback Method
tc	770.19	K	Joback Method
tf	365.94	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.71	J/mol×K	585.65	Joback Method
cpg	405.39	J/mol×K	616.41	Joback Method
cpg	417.49	J/mol×K	647.16	Joback Method
cpg	429.03	J/mol×K	677.92	Joback Method
cpg	440.00	J/mol×K	708.67	Joback Method
cpg	450.41	J/mol×K	739.43	Joback Method
cpg	460.27	J/mol×K	770.19	Joback Method

Sources

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=U352258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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