3-Amino-1-propanol, N,O-diacetyl-

Inchi: InChI=1S/C7H13NO3/c1-6(9)8-4-3-5-11-7(2)10/h3-5H2,1-2H3,(H,8,9)
InchiKey: DPWZYRHWCCZPDJ-UHFFFAOYSA-N
Formula: C7H13NO3
SMILES: CC(=O)NCCCOC(C)=O
Mol. weight [g/mol]: 159.18

Physical Properties

Property code	Value	Unit	Source
gf	-265.39	kJ/mol	Joback Method
hf	-491.72	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-0.58		Crippen Method
logp	0.076		Crippen Method
mcvol	128.480	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1346.60		NIST Webbook
rinpol	1346.60		NIST Webbook
tb	539.89	K	Joback Method
tc	728.58	K	Joback Method
tf	343.40	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.98	J/mol×K	539.89	Joback Method
cpg	310.96	J/mol×K	571.34	Joback Method
cpg	321.46	J/mol×K	602.79	Joback Method
cpg	331.48	J/mol×K	634.24	Joback Method
cpg	341.04	J/mol×K	665.68	Joback Method
cpg	350.12	J/mol×K	697.13	Joback Method
cpg	358.74	J/mol×K	728.58	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=U352255&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