

6-Amino-1-hexanol, N,O-diacetyl-

Inchi:	InChI=1S/C10H19NO3/c1-9(12)11-7-5-3-4-6-8-14-10(2)13/h3-8H2,1-2H3,(H,11,12)
InchiKey:	OKYQCIOPPUJZLL-UHFFFAOYSA-N
Formula:	C10H19NO3
SMILES:	CC(=O)OCCCCCN=C(C)O
Mol. weight [g/mol]:	201.26

Physical Properties

Property code	Value	Unit	Source
hf	-574.33	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	2.086		Crippen Method
mcvol	170.750	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1692.00		NIST Webbook
tb	673.23	K	Joback Method
tc	856.25	K	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=U352301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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

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