O-(Carboxymethyl)hydroxylamine, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C9H18N2O3/c1-4-5-6-13-9(12)7-14-10-8-11(2)3/h8H,4-7H2,1-3H3
InchiKey: KNWPWFIGKVKRHY-UHFFFAOYSA-N
Formula: C9H18N2O3
SMILES: CCCCOC(=O)CON=CN(C)C
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
hf	-456.36	kJ/mol	Joback Method
hvap	52.55	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.851		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
tb	593.15	K	Joback Method
tc	780.15	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=U375781&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