

Glycine, n-[(2-chloroethyl)carbamoyl]-n-nitroso-, ethyl ester	
InChI:	InChI=1S/C7H12CIN3O4/c1-2-15-6(12)5-11(10-14)7(13)9-4-3-8/h2-5H2,1H3,(H,9,13)
InchiKey:	CSJFBJFAUCXAST-UHFFFAOYSA-N
Formula:	C7H12CIN3O4
SMILES:	CCOC(=O)CN(N=O)C(=O)NCCCI
Mol. weight [g/mol]:	237.64
CAS:	60285-28-1

Physical Properties

Property code	Value	Unit	Source
hf	-608.12	kJ/mol	Joback Method
hvap	69.04	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	0.481		Crippen Method
mcvol	162.250	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	653.16	K	Joback Method
tc	842.27	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=C60285281&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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