

Glycine, N-methyl-N-ethoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C8H15NO4/c1-4-12-7(10)6-9(3)8(11)13-5-2/h4-6H2,1-3H3
InchiKey:	VSHIEHLQVBVEMG-UHFFFAOYSA-N
Formula:	C8H15NO4
SMILES:	CCOC(=O)CN(C)C(=O)OCC
Mol. weight [g/mol]:	189.21

Physical Properties

Property code	Value	Unit	Source
gf	-340.58	kJ/mol	Joback Method
hf	-630.52	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.638		Crippen Method
mcvol	148.440	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1307.00		NIST Webbook
tb	547.46	K	Joback Method
tc	729.21	K	Joback Method
tf	356.71	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.47	J/molxK	547.46	Joback Method
cpg	368.63	J/molxK	577.75	Joback Method
cpg	380.29	J/molxK	608.04	Joback Method
cpg	391.45	J/molxK	638.34	Joback Method
cpg	402.10	J/molxK	668.63	Joback Method
cpg	412.23	J/molxK	698.92	Joback Method
cpg	421.86	J/molxK	729.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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