

Glycine, n-methyl-n-methoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C7H13NO4/c1-4-12-6(9)5-8(2)7(10)11-3/h4-5H2,1-3H3
InchiKey:	CMTYJBXWQIYKML-UHFFFAOYSA-N
Formula:	C7H13NO4
SMILES:	CCOC(=O)CN(C)C(=O)OC
Mol. weight [g/mol]:	175.18

Physical Properties

Property code	Value	Unit	Source
af	0.5842		Cheméo Relay (1.0)
gf	-349.00	kJ/mol	Joback Method
hf	-761.05	kJ/mol	Cheméo Relay (1.0)
hfus	22.48	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Cheméo Relay (1.0)
ie	9.21	eV	Cheméo Relay (1.0)
log10ws	-0.23		Cheméo Relay (1.0)
logp	0.248		Crippen Method
mcvol	134.350	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1248.00		NIST Webbook
tb	505.12	K	Cheméo Relay (1.0)
tc	669.68	K	Cheméo Relay (1.0)
tf	274.99	K	Cheméo Relay (1.0)
vc	0.518	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.27	J/mol×K	524.58	Joback Method
cpg	322.52	J/mol×K	555.19	Joback Method
cpg	333.31	J/mol×K	585.80	Joback Method
cpg	343.66	J/mol×K	616.41	Joback Method
cpg	353.54	J/mol×K	647.02	Joback Method
cpg	362.97	J/mol×K	677.63	Joback Method
cpg	371.94	J/mol×K	708.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320602&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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