Glycylglycine ethyl ester

Other names:	Ethyl glycylglycinate
	Glycine, N-glycyl-, ethyl ester
	Ethyl N-glycylglycine
Inchi:	InChI=1S/C6H12N2O3/c1-2-11-6(10)4-8-5(9)3-7/h2-4,7H2,1H3,(H,8,9)
InchiKey:	LFAVEINQLWIXRA-UHFFFAOYSA-N
Formula:	C6H12N2O4
SMILES:	CCOC(=O)CNC(=O)CN
Mol. weight [g/mol]:	176.17
CAS:	627-74-7

Physical Properties

Property code	Value	Unit	Source
chs	-3370.60	kJ/mol	NIST Webbook
gf	-207.36	kJ/mol	Joback Method
hf	-437.29	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	61.93	kJ/mol	Joback Method
log10ws	0.40		Crippen Method
logp	-1.376		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	589.54	K	Joback Method
tc	789.71	K	Joback Method
tf	415.39	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.60	J/mol×K	589.54	Joback Method
cpg	318.74	J/mol×K	622.90	Joback Method
cpg	328.37	J/mol×K	656.26	Joback Method
cpg	337.49	J/mol×K	689.62	Joback Method
cpg	346.10	J/mol×K	722.99	Joback Method

cpg	354.21	J/mol×K	756.35	Joback Method
cpg	361.81	J/mol×K	789.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume