N-(beta-cyanoethyl)glycine ethyl ester

Inchi: InChI=1S/C7H12N2O2/c1-2-11-7(10)6-9-5-3-4-8/h9H,2-3,5-6H2,1H3
InchiKey: SBPUJTNHAUBDKF-UHFFFAOYSA-N
Formula: C7H12N2O2
SMILES: CCOC(=O)CNCCC#N
Mol. weight [g/mol]: 156.18
CAS: 44981-94-4

Physical Properties

Property code	Value	Unit	Source
gf	-3.29	kJ/mol	Joback Method
hf	-214.26	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	57.25	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.053		Crippen Method
mcvol	128.290	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	588.10	K	Joback Method
tc	784.37	K	Joback Method
tf	358.46	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.17	J/mol×K	588.10	Joback Method
cpg	319.19	J/mol×K	620.81	Joback Method
cpg	328.73	J/mol×K	653.52	Joback Method
cpg	337.80	J/mol×K	686.23	Joback Method
cpg	346.41	J/mol×K	718.94	Joback Method
cpg	354.54	J/mol×K	751.66	Joback Method
cpg	362.21	J/mol×K	784.37	Joback Method

Sources

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=C44981944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume