2-Pyrrolidinecarboxylic acid-5-oxo-, ethyl ester

Other names: ethyl pyroglumate (probably ethyl pyroglutamate)
Inchi: InChI=1S/C7H11NO3/c1-2-11-7(10)5-3-4-6(9)8-5/h5H,2-4H2,1H3,(H,8,9)
InchiKey: QYJOOVQLTTVTJY-UHFFFAOYSA-N
Formula: C7H11NO3
SMILES: CCOC(=O)C1CCC(O)=N1
Mol. weight [g/mol]: 157.17

Physical Properties

Property code	Value	Unit	Source
gf	-189.02	kJ/mol	Joback Method
hf	-407.08	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.668		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1447.00		NIST Webbook
tb	601.15	K	Joback Method
tc	805.55	K	Joback Method
tf	397.35	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.33	J/mol×K	601.15	Joback Method
cpg	324.23	J/mol×K	635.22	Joback Method
cpg	335.48	J/mol×K	669.28	Joback Method
cpg	346.09	J/mol×K	703.35	Joback Method
cpg	356.04	J/mol×K	737.41	Joback Method
cpg	365.34	J/mol×K	771.48	Joback Method
cpg	373.97	J/mol×K	805.55	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=U197386&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume