dl-Proline

Other names:	2-Pyrrolidine carboxylic acid
	Proline, DL-
Inchi:	InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)
InchiKey:	ONIBWKKTOPOVIA-UHFFFAOYSA-N
Formula:	C5H9NO2
SMILES:	O=C(O)C1CCCN1
Mol. weight [g/mol]:	115.13
CAS:	609-36-9

Physical Properties

Property code	Value	Unit	Source
chs	-2729.60 ± 0.54	kJ/mol	NIST Webbook
gf	-150.26	kJ/mol	Joback Method
hf	-313.05	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	-0.177		Crippen Method
mcvol	87.870	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
tb	523.68	K	Joback Method
tc	729.91	K	Joback Method
tf	372.79	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.66	J/mol×K	523.68	Joback Method
cpg	211.92	J/mol×K	558.05	Joback Method
cpg	221.63	J/mol×K	592.42	Joback Method
cpg	230.81	J/mol×K	626.80	Joback Method
cpg	239.45	J/mol×K	661.17	Joback Method
cpg	247.59	J/mol×K	695.54	Joback Method

cpg	255.23	J/mol×K	729.91	Joback Method

Sources

THE STANDARD ENTHALPIES OF FORMATION OF PROLINE ISOMERS:	https://www.doi.org/10.1016/j.tca.2012.02.035
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=C609369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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