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

Physical Properties

Property code	Value	Unit	Source
chs	-2729.60 ± 0.54	kJ/mol	NIST Webbook
hf	-374.73	kJ/mol	Cheméo Relay (1.0)
hfus	17.92	kJ/mol	Joback Method
ie	8.94	eV	Cheméo Relay (1.0)
logp	-0.177		Crippen Method
mcvol	87.870	ml/mol	McGowan 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
THE STANDARD ENTHALPIES OF FORMATION OF PROLINE ISOMERS:	https://www.doi.org/10.1016/j.tca.2012.02.035
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609369&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume