DL-5-Oxoproline

Other names:	DL-Pyroglutamic acid
	2-Pyrrolidone-5-carboxylic acid
	DL-5-Oxoproline
	5-oxo-DL-proline
Inchi:	InChI=1S/C5H7NO3/c7-4-2-1-3(6-4)5(8)9/h3H,1-2H2,(H,6,7)(H,8,9)
InchiKey:	ODHCTXKNWHHXJC-UHFFFAOYSA-N
Formula:	C5H7NO3
SMILES:	O=C1CCC(C(=O)O)N1
Mol. weight [g/mol]:	129.11

Physical Properties

Property code	Value	Unit	Source
hfus	17.43	kJ/mol	Joback Method
logp	-0.650		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
tb	547.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.24	J/mol×K	591.50	Joback Method
cpg	230.15	J/mol×K	628.20	Joback Method
cpg	239.54	J/mol×K	664.90	Joback Method
cpg	248.40	J/mol×K	701.60	Joback Method
cpg	256.72	J/mol×K	738.30	Joback Method
cpg	264.47	J/mol×K	775.00	Joback Method
cpg	271.63	J/mol×K	811.70	Joback Method
hsubt	133.00 ± 1.00	kJ/mol	405.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C149871&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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