pentaglycine

Inchi: InChI=1S/C10H17N5O6/c11-1-6(16)12-2-7(17)13-3-8(18)14-4-9(19)15-5-10(20)21/h1-5,1
InchiKey: MXHCPCSDRGLRER-UHFFFAOYSA-N
Formula: C10H17N5O6
SMILES: NCC(=O)NCC(=O)NCC(=O)NCC(=O)NCC(=O)O
Mol. weight [g/mol]: 303.27

Physical Properties

Property code	Value	Unit	Source
hf	-1056.37	kJ/mol	Cheméo Relay (1.0)
hfus	59.33	kJ/mol	Joback Method
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-0.71		Cheméo Relay (1.0)
logp	-4.505		Crippen Method
mcvol	215.380	ml/mol	McGowan Method
tf	495.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.95	J/mol×K	1062.94	Joback Method
cpg	699.95	J/mol×K	1102.76	Joback Method
cpg	705.06	J/mol×K	1142.59	Joback Method
cpg	709.34	J/mol×K	1182.41	Joback Method
cpg	712.82	J/mol×K	1222.23	Joback Method
cpg	715.55	J/mol×K	1262.05	Joback Method
cpg	717.59	J/mol×K	1301.88	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C7093676&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point