DL-LEUCYLGLYCINE

Other names: dl-Leucylglycine
Glycine, N-DL-leucyl-
Inchi: InChI=1S/C8H16N2O3/c1-5(2)3-6(9)8(13)10-4-7(11)12/h5-6H,3-4,9H2,1-2H3,(H,10,13)(H
InchiKey: LESXFEZIFXFIQR-UHFFFAOYSA-N
Formula: C8H16N2O3
SMILES: CC(C)CC(N)C(=O)NCC(=O)O
Mol. weight [g/mol]: 188.23

Physical Properties

Property code	Value	Unit	Source
chs	-4574.80 ± 1.20	kJ/mol	NIST Webbook
chs	-4586.60 ± 0.60	kJ/mol	NIST Webbook
hfs	-859.90 ± 1.30	kJ/mol	NIST Webbook
hfus	27.01	kJ/mol	Joback Method
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-0.88		Cheméo Relay (1.0)
logp	-0.439		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
ss	281.20	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.76	J/mol×K	704.18	Joback Method
cpg	439.99	J/mol×K	736.42	Joback Method
cpg	449.61	J/mol×K	768.67	Joback Method
cpg	458.65	J/mol×K	800.91	Joback Method
cpg	467.13	J/mol×K	833.15	Joback Method
cpg	475.06	J/mol×K	865.40	Joback Method
cpg	482.46	J/mol×K	897.64	Joback Method
cps	255.64	J/mol×K	297.10	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=C615827&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hfs:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions