

D-Leucylglycylglycine

Other names:	Glycine, N-(N-D-leucylglycyl)- N-(N-D-leucylglycyl)glycine
Inchi:	InChI=1S/C10H19N3O4/c1-6(2)3-7(11)10(17)13-4-8(14)12-5-9(15)16/h6-7H,3-5,11H2,1-
InchiKey:	VWHGTYCRDRBSFI-ZETCQYMHSA-N
Formula:	C10H19N3O4
SMILES:	CC(C)CC(N)C(=O)NCC(=O)NCC(=O)O
Mol. weight [g/mol]:	245.28
CAS:	18625-22-4

Physical Properties

Property code	Value	Unit	Source
chs	-5592.50	kJ/mol	NIST Webbook
gf	-249.91	kJ/mol	Joback Method
hf	-609.53	kJ/mol	Joback Method
hfus	38.89	kJ/mol	Joback Method
hvap	97.51	kJ/mol	Joback Method
log10ws	-0.34		Crippen Method
logp	-1.323		Crippen Method
mcvol	192.280	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	853.98	K	Joback Method
tc	1056.80	K	Joback Method
tf	571.65	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.64	J/molxK	853.98	Joback Method
cpg	604.41	J/molxK	887.78	Joback Method
cpg	613.46	J/molxK	921.59	Joback Method
cpg	621.80	J/molxK	955.39	Joback Method
cpg	629.48	J/molxK	989.19	Joback Method
cpg	636.51	J/molxK	1022.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C18625224&Units=SI

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

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