2,5-Piperazinedione

Other names:	.alpha.,.gamma.-diacipiperazine
	2,5-Diketopiperazine
	2,5-Dioxopiperazine
	Cyclic(glycylglycyl)
	Cyclo(glycylglycyl)
	Cyclodiglycine
	Cycloglycylglycine
	Diglycolyl diamide
	Diketopiperazine
	Glycine, N-glycyl-, cyclic peptide
	Glycine, bimol. cyclic peptide
	Glycylglycine lactam
	NSC 26345
	Piperazine-2,5-dione
	«alpha»,«gamma»-Diacipiperazine
	Â«alphaÂ»,Â«gammaÂ»-Diacipiperazine
Inchi:	InChI=1S/C4H6N2O2/c7-3-1-5-4(8)2-6-3/h1-2H2,(H,5,8)(H,6,7)
InchiKey:	BXRNXXXXHLBUKK-UHFFFAOYSA-N
Formula:	C4H6N2O2
SMILES:	O=C1CNC(=O)CN1
Mol. weight [g/mol]:	114.10
CAS:	106-57-0

Physical Properties

Property code	Value	Unit	Source
chs	-1992.00	kJ/mol	NIST Webbook
chs	-1993.00	kJ/mol	NIST Webbook
chs	-1990.10 ± 0.20	kJ/mol	NIST Webbook
chs	-1985.00 ± 1.30	kJ/mol	NIST Webbook
gf	-54.80	kJ/mol	Joback Method
hf	-251.01	kJ/mol	Joback Method
hfs	-446.00 ± 1.30	kJ/mol	NIST Webbook
hfus	15.08	kJ/mol	Joback Method
hvap	47.25	kJ/mol	Joback Method
log10ws	-0.83		Aqueous Solubility Prediction Method
logp	-1.768		Crippen Method

mcvol	79.460	ml/mol	McGowan Method
pc	6461.89	kPa	Joback Method
ss	145.60	J/mol×K	NIST Webbook
ss	145.50	J/mol×K	NIST Webbook
tb	547.88	K	Joback Method
tc	814.53	K	Joback Method
tf	492.96	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.22	J/mol×K	681.20	Joback Method
cpg	198.97	J/mol×K	636.76	Joback Method
cpg	239.58	J/mol×K	814.53	Joback Method
cpg	230.64	J/mol×K	770.09	Joback Method
cpg	220.81	J/mol×K	725.65	Joback Method
cpg	187.18	J/mol×K	592.32	Joback Method
cpg	174.96	J/mol×K	547.88	Joback Method
cps	133.90	J/mol×K	298.15	NIST Webbook
cps	134.00	J/mol×K	298.15	NIST Webbook
hsubt	103.80	kJ/mol	431.50	NIST Webbook
psub	4.70e-04	kPa	437.19	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	5.48e-04	kPa	439.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	6.46e-04	kPa	441.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine

psub	9.91e-05	kPa	419.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.18e-04	kPa	421.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.40e-04	kPa	423.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.68e-04	kPa	425.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.96e-04	kPa	427.10	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	2.32e-04	kPa	429.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	2.90e-04	kPa	431.17	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.30e-04	kPa	433.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.82e-04	kPa	435.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine

psub	4.59e-04	kPa	437.19	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	5.19e-04	kPa	439.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	6.27e-04	kPa	441.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	9.65e-05	kPa	419.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.14e-04	kPa	421.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.37e-04	kPa	423.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.56e-04	kPa	425.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.88e-04	kPa	427.10	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	

psub	2.26e-04	kPa	429.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	2.57e-04	kPa	431.17	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.20e-04	kPa	433.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.80e-04	kPa	435.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	5.20e-04	kPa	439.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	6.26e-04	kPa	441.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.90e-04	kPa	435.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.47e-04	kPa	433.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	2.73e-04	kPa	431.17	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine

psub	2.36e-04	kPa	429.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.62e-04	kPa	425.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.41e-04	kPa	423.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.19e-04	kPa	421.11	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.01e-04	kPa	419.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.95e-04	kPa	427.10	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Ammonium based ionic liquids act as compatible solvents for glycine peptides:	https://www.doi.org/10.1016/j.jct.2012.07.009
Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine:	https://www.doi.org/10.1016/j.jct.2012.10.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities of aqueous solutions containing model compounds of amino acids and ionic salts at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2006.11.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Thermodynamic contributions of peptide backbone unit from water to biocompatible ionic liquids at T = 298.15 K:

https://www.doi.org/10.1016/j.jct.2011.09.017

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
psub:	Sublimation pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume