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	-1985.00 ± 1.30	kJ/mol	NIST Webbook
chs	-1992.00	kJ/mol	NIST Webbook
chs	-1993.00	kJ/mol	NIST Webbook
chs	-1990.10 ± 0.20	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	174.96	J/mol×K	547.88	Joback Method
cpg	187.18	J/mol×K	592.32	Joback Method
cpg	198.97	J/mol×K	636.76	Joback Method
cpg	210.22	J/mol×K	681.20	Joback Method
cpg	220.81	J/mol×K	725.65	Joback Method
cpg	230.64	J/mol×K	770.09	Joback Method
cpg	239.58	J/mol×K	814.53	Joback Method
cps	134.00	J/mol×K	298.15	NIST Webbook
cps	133.90	J/mol×K	298.15	NIST Webbook
hsubt	103.80	kJ/mol	431.50	NIST Webbook
psub	9.91e-05	kPa	419.16	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	1.41e-04	kPa	423.15	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	1.95e-04	kPa	427.10	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	2.73e-04	kPa	431.17	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	3.90e-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	5.48e-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	1.01e-04	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	4.70e-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

Sources

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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106570&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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