3,6-Dimethylpiperazine-2,5-dione

Other names:	2,5-Piperazinedione, 3,6-dimethyl-
	3,6-Dimethyl-2,5-piperazinedione
	3,6-Dimethyldiketopiperazine
	Alanine anhydride
	dl-Alanine anhydride
Inchi:	InChI=1S/C6H10N2O2/c1-3-5(9)8-4(2)6(10)7-3/h3-4H,1-2H3,(H,7,10)(H,8,9)
InchiKey:	WWISPHBAYBECQZ-UHFFFAOYSA-N
Formula:	C6H10N2O2
SMILES:	CC1NC(=O)C(C)NC1=O
Mol. weight [g/mol]:	142.16
CAS:	5625-46-7

Physical Properties

Property code	Value	Unit	Source
chs	-3300.00	kJ/mol	NIST Webbook
chs	-3301.10	kJ/mol	NIST Webbook
gf	-53.38	kJ/mol	Joback Method
hf	-332.97	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	51.08	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	-0.991		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	584.30	K	Joback Method
tc	839.12	K	Joback Method
tf	507.02	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.31	J/mol×K	584.30	Joback Method
cpg	285.07	J/mol×K	626.77	Joback Method

cpg	300.14	J/mol×K	669.24	Joback Method
cpg	314.42	J/mol×K	711.71	Joback Method
cpg	327.78	J/mol×K	754.18	Joback Method
cpg	340.11	J/mol×K	796.65	Joback Method
cpg	351.30	J/mol×K	839.12	Joback Method
psub	1.42e-04	kPa	390.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.49e-04	kPa	390.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.79e-04	kPa	392.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	2.16e-04	kPa	394.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	2.67e-04	kPa	396.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.25e-04	kPa	398.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.88e-04	kPa	400.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	4.63e-04	kPa	402.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine

psub	5.63e-04	kPa	404.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	6.93e-04	kPa	406.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	8.21e-04	kPa	408.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	9.77e-04	kPa	410.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.26e-04	kPa	388.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.16e-04	kPa	388.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	1.71e-04	kPa	392.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	2.60e-04	kPa	396.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	

psub	3.09e-04	kPa	398.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	3.87e-04	kPa	400.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	4.54e-04	kPa	402.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	5.43e-04	kPa	404.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	6.96e-04	kPa	406.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	8.18e-04	kPa	408.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	9.55e-04	kPa	410.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.16e-04	kPa	388.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine
psub	1.40e-04	kPa	390.16	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine

psub	2.12e-04	kPa	394.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	2.47e-04	kPa	396.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	2.98e-04	kPa	398.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	3.71e-04	kPa	400.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	4.36e-04	kPa	402.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	6.77e-04	kPa	406.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	7.85e-04	kPa	408.14	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	
psub	9.27e-04	kPa	410.15	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5625467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Volumetric, Acoustic, and Refractometric Study of Cyclic Alanylalanine in Aqueous Cobalt Chloride Solutions at Temperatures T = (293.15 to 313.15) K:	https://www.doi.org/10.1021/je3009123
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume