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	-3301.10	kJ/mol	NIST Webbook
chs	-3300.00	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	351.30	J/mol×K	839.12	Joback Method
cpg	340.11	J/mol×K	796.65	Joback Method

cpg	327.78	J/mol×K	754.18	Joback Method
cpg	314.42	J/mol×K	711.71	Joback Method
cpg	300.14	J/mol×K	669.24	Joback Method
cpg	285.07	J/mol×K	626.77	Joback Method
cpg	269.31	J/mol×K	584.30	Joback Method
psub	6.96e-04	kPa	406.14	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	1.42e-04	kPa	390.16	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	4.63e-04	kPa	402.13	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	
psub	3.88e-04	kPa	400.13	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	2.67e-04	kPa	396.14	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	1.79e-04	kPa	392.15	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	1.16e-04	kPa	388.13	Experimental and computational study on the energetics of the cyclic anhydrides of glycine and alanine	

Sources

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
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

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