(l,l)-cis-3,6-Dimethylpiperazine-2,5-dione

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)/t3-,4-/m1/s1
InchiKey: WWISPHBAYBECQZ-QWWZWVQMSA-N
Formula: C6H10N2O2
SMILES: CC1NC(=O)C(C)NC1=O
Mol. weight [g/mol]: 142.16
CAS: 5845-61-4

Physical Properties

Property code	Value	Unit	Source
chs	-3292.80 ± 0.30	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

Sources

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=C5845614&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume