

2,5-Piperazinedione, 3,6-dimethyl-, trans-

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+
InchiKey:	WWISPHBAYBECQZ-ZXZARUISSA-N
Formula:	C6H10N2O2
SMILES:	CC1NC(=O)C(C)NC1=O
Mol. weight [g/mol]:	142.16
CAS:	35590-65-9

Physical Properties

Property code	Value	Unit	Source
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/molxK	584.30	Joback Method
cpg	285.07	J/molxK	626.77	Joback Method
cpg	300.14	J/molxK	669.24	Joback Method
cpg	314.42	J/molxK	711.71	Joback Method
cpg	327.78	J/molxK	754.18	Joback Method
cpg	340.11	J/molxK	796.65	Joback Method
cpg	351.30	J/molxK	839.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35590659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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