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

Inchi: InChI=1S/C10H18N2O2/c1-5(2)7-9(13)12-8(6(3)4)10(14)11-7/h5-8H,1-4H3,(H,11,14)(H,1

InchiKey: QGMAWEIDGADSAC-YUMQZZPRSA-N

Formula: C10H18N2O2

SMILES: CC(C)C1NC(=O)C(C(C)C)NC1=O

Mol. weight [g/mol]: 198.26

CAS: 19943-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-24.58	kJ/mol	Joback Method
hf	-426.09	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	59.21	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.282		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	674.94	K	Joback Method
tc	918.34	K	Joback Method
tf	522.10	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.86	J/mol×K	674.94	Joback Method
cpg	491.41	J/mol×K	715.51	Joback Method
cpg	509.71	J/mol×K	756.07	Joback Method
cpg	526.67	J/mol×K	796.64	Joback Method
cpg	542.22	J/mol×K	837.21	Joback Method
cpg	556.27	J/mol×K	877.78	Joback Method
cpg	568.75	J/mol×K	918.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19943169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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