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

Inchi: InChI=1S/C12H22N2O2/c1-7(2)5-9-11(15)14-10(6-8(3)4)12(16)13-9/h7-10H,5-6H2,1-4H
InchiKey: XWYXUMDVQIOAPR-NXEZZACHSA-N
Formula: C12H22N2O2
SMILES: CC(C)CC1NC(=O)C(CC(C)C)NC1=O
Mol. weight [g/mol]: 226.32
CAS: 16679-67-7

Physical Properties

Property code	Value	Unit	Source
gf	-7.74	kJ/mol	Joback Method
hf	-467.37	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	63.66	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.062		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
tb	720.70	K	Joback Method
tc	954.38	K	Joback Method
tf	544.64	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.34	J/mol×K	720.70	Joback Method
cpg	601.42	J/mol×K	759.65	Joback Method
cpg	620.10	J/mol×K	798.59	Joback Method
cpg	637.32	J/mol×K	837.54	Joback Method
cpg	653.00	J/mol×K	876.48	Joback Method
cpg	667.10	J/mol×K	915.43	Joback Method
cpg	679.55	J/mol×K	954.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C16679677&Units=SI

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