2,5-Piperazinedione, 3-benzyl-6-isopropyl-

Other names: 3-Benzyl-6-isopropyl-2,5-piperazinedione
Inchi: InChI=1S/C14H18N2O2/c1-9(2)12-14(18)15-11(13(17)16-12)8-10-6-4-3-5-7-10/h3-7,9,11
InchiKey: OQQPOHUVAQPSHJ-UHFFFAOYSA-N
Formula: C14H18N2O2
SMILES: CC(C)C1NC(=O)C(Cc2ccccc2)NC1=O
Mol. weight [g/mol]: 246.30
CAS: 14474-71-6

Physical Properties

Property code	Value	Unit	Source
chs	-7689.00 ± 4.00	kJ/mol	NIST Webbook
gf	123.95	kJ/mol	Joback Method
hf	-266.84	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	70.78	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	0.868		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	793.58	K	Joback Method
tc	1056.68	K	Joback Method
tf	608.60	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.92	J/mol×K	793.58	Joback Method
cpg	624.60	J/mol×K	837.43	Joback Method
cpg	641.30	J/mol×K	881.28	Joback Method
cpg	655.95	J/mol×K	925.13	Joback Method
cpg	668.49	J/mol×K	968.98	Joback Method
cpg	678.85	J/mol×K	1012.83	Joback Method
cpg	686.97	J/mol×K	1056.68	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=C14474716&Units=SI

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