2,5-PIPERAZINEDIONE, 3-(PHENYLMETHYL)-

Other names: 3-Benzoylpiperazine-2,5-dione
Piperazine-2,5-dione, 3-benzyl-
3-Benzyl-2,5-piperazinedione
3-Benzyl-piperazine-2,5-dione
Inchi: InChI=1S/C11H12N2O2/c14-10-7-12-11(15)9(13-10)6-8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,1
InchiKey: UZOJHXFWJFSFAI-UHFFFAOYSA-N
Formula: C11H12N2O2
SMILES: O=C1CNC(=O)C(Cc2ccccc2)N1
Mol. weight [g/mol]: 204.23

Physical Properties

Property code	Value	Unit	Source
chs	-5698.00 ± 2.00	kJ/mol	NIST Webbook
hfus	28.32	kJ/mol	Joback Method
logp	-0.156		Crippen Method
mcvol	154.330	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.33	J/mol×K	730.05	Joback Method
cpg	454.82	J/mol×K	776.25	Joback Method
cpg	470.61	J/mol×K	822.44	Joback Method
cpg	484.63	J/mol×K	868.64	Joback Method
cpg	496.79	J/mol×K	914.83	Joback Method
cpg	507.02	J/mol×K	961.03	Joback Method
cpg	515.23	J/mol×K	1007.22	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5037752&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume