2,5-PIPERAZINEDIONE, 3-METHYL-6-(PHENYLMETHYL)-

Other names: 3-Benzyl-6-methyl-2,5-piperazinedione
Inchi: InChI=1S/C12H14N2O2/c1-8-11(15)14-10(12(16)13-8)7-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1
InchiKey: CNXWPOWVDIUTPS-UHFFFAOYSA-N
Formula: C12H14N2O2
SMILES: CC1NC(=O)C(Cc2ccccc2)NC1=O
Mol. weight [g/mol]: 218.26

Physical Properties

Property code	Value	Unit	Source
chs	-6351.00 ± 3.00	kJ/mol	NIST Webbook
hfus	31.98	kJ/mol	Joback Method
logp	0.232		Crippen Method
mcvol	168.420	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.45	J/mol×K	748.26	Joback Method
cpg	512.75	J/mol×K	793.35	Joback Method
cpg	529.25	J/mol×K	838.45	Joback Method
cpg	543.87	J/mol×K	883.54	Joback Method
cpg	556.52	J/mol×K	928.63	Joback Method
cpg	567.13	J/mol×K	973.73	Joback Method
cpg	575.60	J/mol×K	1018.82	Joback Method

Sources

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=C14474783&Units=SI

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

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