

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
CAS:	5037-75-2

Physical Properties

Property code	Value	Unit	Source
chs	-5698.00 ± 2.00	kJ/mol	NIST Webbook
gf	108.84	kJ/mol	Joback Method
hf	-179.30	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	-0.156		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	730.05	K	Joback Method
tc	1007.22	K	Joback Method
tf	594.03	K	Joback Method
vc	0.565	m ³ /kmol	Joback 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

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=C5037752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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