

2,5-Piperazinedione, 3,6-bis(phenylmethyl)-

Other names:

Dibenzyl-3,6-dione-2,5-piperazine
Dibenzyl-3, 6-dioxo-2, 5-piperazine
2,5-Piperazinedione, 3,6-dibenzyl-
3,6-Dibenzyl-2,5-piperazinedione
Phenylalanine anhydride
Phenylalanylhydride

Inchi:

InChI=1S/C18H18N2O2/c21-17-15(11-13-7-3-1-4-8-13)19-18(22)16(20-17)12-14-9-5-2-6

InchiKey:

JUAPMRSLDANLAS-UHFFFAOYSA-N

Formula:

C18H18N2O2

SMILES:

O=C1NC(Cc2ccccc2)C(=O)NC1Cc1ccccc1

Mol. weight [g/mol]:

294.35

CAS:

2308-61-4

Physical Properties

Property code	Value	Unit	Source
chs	-9368.02 ± 0.92	kJ/mol	NIST Webbook
gf	272.48	kJ/mol	Joback Method
hf	-107.59	kJ/mol	Joback Method
hfus	41.56	kJ/mol	Joback Method
hvap	82.34	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	1.455		Crippen Method
mcvol	229.200	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	912.22	K	Joback Method
tc	1191.94	K	Joback Method
tf	695.10	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.74	J/mol×K	912.22	Joback Method
cpg	752.02	J/mol×K	958.84	Joback Method

cpg	764.70	J/mol×K	1005.46	Joback Method
cpg	774.76	J/mol×K	1052.08	Joback Method
cpg	782.15	J/mol×K	1098.70	Joback Method
cpg	786.85	J/mol×K	1145.32	Joback Method
cpg	788.82	J/mol×K	1191.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C2308614&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

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