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]: 218.25
CAS: 14474-78-3

Physical Properties

Property code	Value	Unit	Source
chs	-6351.00 ± 3.00	kJ/mol	NIST Webbook
gf	109.55	kJ/mol	Joback Method
hf	-220.28	kJ/mol	Joback Method
hfus	31.98	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	0.232		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	748.26	K	Joback Method
tc	1018.82	K	Joback Method
tf	601.06	K	Joback Method
vc	0.620	m3/kmol	Joback 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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14474783&Units=SI
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

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