6Alpha-(p-nitrobenzamido)-3alpha,5-cyclo-5alpha

Inchi: InChI=1S/C26H32N2O4/c1-24-11-10-20-18(19(24)7-8-22(24)29)13-21(26-14-16(26)9-12
InchiKey: JDBQTVZYXDVVOM-HFRMBQMUSA-N
Formula: C26H32N2O4
SMILES: CC12CCC3C(CC(NC(=O)c4ccc([N+](=O)[O-])cc4)C45CC4CCC35C)C1CCC2=O
Mol. weight [g/mol]: 436.54
CAS: 103064-86-4

Physical Properties

Property code	Value	Unit	Source
gf	384.20	kJ/mol	Joback Method
hf	-226.10	kJ/mol	Joback Method
hfus	45.11	kJ/mol	Joback Method
hvap	105.96	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	4.915		Crippen Method
mcvol	329.680	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
tb	1178.59	K	Joback Method
tc	1460.70	K	Joback Method
tf	877.78	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.81	J/mol×K	1178.59	Joback Method
cpg	1507.29	J/mol×K	1225.61	Joback Method
cpg	1578.21	J/mol×K	1272.63	Joback Method
cpg	1657.49	J/mol×K	1319.65	Joback Method
cpg	1746.02	J/mol×K	1366.66	Joback Method
cpg	1844.72	J/mol×K	1413.68	Joback Method
cpg	1954.49	J/mol×K	1460.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103064864&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

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