5-Cyclo-5alpha-androstan-6beta-ol, 17-ethylenedioxy-3alpha, p-nitrobenzoate

Inchi: InChI=1S/C28H35NO6/c1-25-10-7-18-16-27(18,25)23(35-24(30)17-3-5-19(6-4-17)29(31)

InchiKey: XXFZHDNVDLTTSI-UHFFFAOYSA-N

Formula: C28H35NO6

SMILES: CC12CCC3C(CC(OC(=O)c4ccc([N+](=O)[O-])cc4)C45CC4CCC35C)C1CCC21OCCO1

Mol. weight [g/mol]: 481.58

Physical Properties

Property code	Value	Unit	Source
gf	200.16	kJ/mol	Joback Method
hf	-497.49	kJ/mol	Joback Method
hfus	52.56	kJ/mol	Joback Method
hvap	110.09	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.516		Crippen Method
mcvol	353.060	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
tb	1193.93	K	Joback Method
tc	1478.74	K	Joback Method
tf	893.13	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1627.54	J/mol×K	1193.93	Joback Method
cpg	1712.91	J/mol×K	1241.40	Joback Method
cpg	1809.32	J/mol×K	1288.87	Joback Method
cpg	1917.98	J/mol×K	1336.33	Joback Method
cpg	2040.09	J/mol×K	1383.80	Joback Method
cpg	2176.86	J/mol×K	1431.27	Joback Method
cpg	2329.48	J/mol×K	1478.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006129&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