11-Deoxycorticosterone, pivalate

Other names: desoxycortone pivalate
Inchi: InChI=1S/C26H38O4/c1-24(2,3)23(29)30-15-22(28)21-9-8-19-18-7-6-16-14-17(27)10-12-
InchiKey: VVOIQBFMTVCINR-UHFFFAOYSA-N
Formula: C26H38O4
SMILES: CC(C)(C)C(=O)OCC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 414.58
CAS: 808-48-0

Physical Properties

Property code	Value	Unit	Source
gf	-138.12	kJ/mol	Joback Method
hf	-787.29	kJ/mol	Joback Method
hfus	32.00	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.293		Crippen Method
mcvol	340.040	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
tb	1032.62	K	Joback Method
tc	1281.68	K	Joback Method
tf	682.27	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1303.94	J/mol×K	1032.62	Joback Method
cpg	1336.07	J/mol×K	1074.13	Joback Method
cpg	1369.49	J/mol×K	1115.64	Joback Method
cpg	1404.58	J/mol×K	1157.15	Joback Method
cpg	1441.78	J/mol×K	1198.66	Joback Method
cpg	1481.47	J/mol×K	1240.17	Joback Method
cpg	1524.07	J/mol×K	1281.68	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=C808480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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