

Allopregnane-7«alpha»,11«alpha»-diol-3,20-dione

Inchi: InChI=1S/C21H32O4/c1-11(22)14-4-5-15-18-16(24)9-12-8-13(23)6-7-20(12,2)19(18)17(2)
InchiKey: OUDYGQOKBCRPKZ-DOCSSMEGSA-N
Formula: C21H32O4
SMILES: CC(=O)C1CCC2C3C(O)CC4CC(=O)CCC4(C)C3C(O)CC12C
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-266.24	kJ/mol	Joback Method
hf	-842.33	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	103.36	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.745		Crippen Method
mcvol	278.190	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	1011.37	K	Joback Method
tc	1244.02	K	Joback Method
tf	646.98	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1111.86	J/molxK	1011.37	Joback Method
cpg	1138.99	J/molxK	1050.14	Joback Method
cpg	1166.99	J/molxK	1088.92	Joback Method
cpg	1196.16	J/molxK	1127.69	Joback Method
cpg	1226.78	J/molxK	1166.47	Joback Method
cpg	1259.15	J/molxK	1205.24	Joback Method
cpg	1293.56	J/molxK	1244.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U251151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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