3«alpha»-5-Cyclo-ergosta-7,22-dien-6-one

Inchi: InChI=1S/C28H42O/c1-17(2)18(3)7-8-19(4)22-9-10-23-21-15-25(29)28-16-20(28)11-14-2
InchiKey: MDLVGBWIRYDJQI-AXOZAPSRSA-N
Formula: C28H42O
SMILES: CC(C)C(C)C=CC(C)C1CCC2C3=CC(=O)C45CC4CCC5(C)C3CCC21C
Mol. weight [g/mol]: 394.63

Physical Properties

Property code	Value	Unit	Source
gf	403.18	kJ/mol	Joback Method
hf	-254.54	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	7.229		Crippen Method
mcvol	344.050	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	3825.00		NIST Webbook
tb	948.46	K	Joback Method
tc	1189.98	K	Joback Method
tf	582.62	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.93	J/mol×K	948.46	Joback Method
cpg	1326.36	J/mol×K	988.71	Joback Method
cpg	1366.11	J/mol×K	1028.97	Joback Method
cpg	1408.74	J/mol×K	1069.22	Joback Method
cpg	1454.85	J/mol×K	1109.47	Joback Method
cpg	1505.04	J/mol×K	1149.73	Joback Method
cpg	1559.89	J/mol×K	1189.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418774&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume