

Pregnenolone palmitate

Inchi:	InChI=1S/C37H62O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-35(39)40-30-23-25-36(3
InchiKey:	FOZPTVPLEKIYFC-QSKSOYRKSA-N
Formula:	C37H62O3
SMILES:	CCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC32)C1
Mol. weight [g/mol]:	554.89

Physical Properties

Property code	Value	Unit	Source
gf	66.54	kJ/mol	Joback Method
hf	-888.22	kJ/mol	Joback Method
hfus	69.46	kJ/mol	Joback Method
hvap	112.09	kJ/mol	Joback Method
log10ws	-11.55		Crippen Method
logp	10.547		Crippen Method
mcvol	493.460	ml/mol	McGowan Method
pc	623.75	kPa	Joback Method
rinsol	4350.00		NIST Webbook
tb	1215.04	K	Joback Method
tc	1507.20	K	Joback Method
tf	731.36	K	Joback Method
vc	1.905	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2079.95	J/mol×K	1215.04	Joback Method
cpg	2137.78	J/mol×K	1263.73	Joback Method
cpg	2199.59	J/mol×K	1312.43	Joback Method
cpg	2266.16	J/mol×K	1361.12	Joback Method
cpg	2338.24	J/mol×K	1409.81	Joback Method
cpg	2416.57	J/mol×K	1458.51	Joback Method
cpg	2501.93	J/mol×K	1507.20	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164155&Units=SI

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
mccvol:	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

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