

5A-Pregnanolone palmitate

Inchi:	InChI=1S/C37H64O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-35(39)40-30-23-25-36(3
InchiKey:	KMUSMBQUDXLHDP-JKXKYAFFSA-N
Formula:	C37H64O3
SMILES:	CCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=O)CCC32)C1
Mol. weight [g/mol]:	556.90

Physical Properties

Property code	Value	Unit	Source
gf	38.50	kJ/mol	Joback Method
hf	-954.87	kJ/mol	Joback Method
hfus	69.70	kJ/mol	Joback Method
hvap	110.83	kJ/mol	Joback Method
log10ws	-11.45		Crippen Method
logp	10.627		Crippen Method
mcvol	497.760	ml/mol	McGowan Method
pc	607.26	kPa	Joback Method
rinqol	4355.00		NIST Webbook
tb	1206.23	K	Joback Method
tc	1496.16	K	Joback Method
tf	713.84	K	Joback Method
vc	1.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2112.46	J/molxK	1206.23	Joback Method
cpg	2168.95	J/molxK	1254.55	Joback Method
cpg	2228.99	J/molxK	1302.87	Joback Method
cpg	2293.31	J/molxK	1351.19	Joback Method
cpg	2362.64	J/molxK	1399.52	Joback Method
cpg	2437.72	J/molxK	1447.84	Joback Method
cpg	2519.29	J/molxK	1496.16	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=R164135&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
hvac:	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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