5A-Pregnanolone oleate

Inchi: InChI=1S/C39H66O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-37(41)42-32-25-2
InchiKey: VRMZKDGHPVGVHQ-WEOJVLFXSA-N
Formula: C39H66O3
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=O)CCC32)
Mol. weight [g/mol]: 582.94

Physical Properties

Property code	Value	Unit	Source
gf	135.56	kJ/mol	Joback Method
hf	-878.93	kJ/mol	Joback Method
hfus	75.08	kJ/mol	Joback Method
hvap	115.24	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	11.184		Crippen Method
mcvol	521.640	ml/mol	McGowan Method
pc	567.43	kPa	Joback Method
rinpol	4585.00		NIST Webbook
tb	1256.15	K	Joback Method
tc	1569.71	K	Joback Method
tf	731.30	K	Joback Method
vc	2.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2255.89	J/mol×K	1256.15	Joback Method
cpg	2324.66	J/mol×K	1308.41	Joback Method
cpg	2399.01	J/mol×K	1360.67	Joback Method
cpg	2479.93	J/mol×K	1412.93	Joback Method
cpg	2568.41	J/mol×K	1465.19	Joback Method
cpg	2665.44	J/mol×K	1517.45	Joback Method
cpg	2772.02	J/mol×K	1569.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164120&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
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
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