

5A-Pregnanolone myristate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C35H60O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-33(37)38-28-21-23-34(3)27(25

FAOSMPQSPCIQNT-WCQWLXOCSA-N

C35H60O3

CCCCCCCCCCCCC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=O)CCC32)C1

528.85

Physical Properties

Property code	Value	Unit	Source
gf	21.66	kJ/mol	Joback Method
hf	-913.59	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	106.38	kJ/mol	Joback Method
log10ws	-10.61		Crippen Method
logp	9.847		Crippen Method
mcvol	469.580	ml/mol	McGowan Method
pc	669.08	kPa	Joback Method
rinpol	4140.00		NIST Webbook
rinpol	4140.00		NIST Webbook
tb	1160.47	K	Joback Method
tc	1428.15	K	Joback Method
tf	691.30	K	Joback Method
vc	1.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1952.21	J/mol×K	1160.47	Joback Method
cpg	2000.36	J/mol×K	1205.08	Joback Method
cpg	2050.97	J/mol×K	1249.70	Joback Method
cpg	2104.62	J/mol×K	1294.31	Joback Method
cpg	2161.87	J/mol×K	1338.92	Joback Method
cpg	2223.29	J/mol×K	1383.54	Joback Method
cpg	2289.45	J/mol×K	1428.15	Joback Method

Sources

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=R164115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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