

Acanthasterol acetate

Inchi:

InChI=1S/C32H52O2/c1-19(2)21(4)32(8)18-29(32)20(3)26-11-12-27-25-10-9-23-17-24(3)

InchiKey:

DMAVMYPLZOJVPK-XDSQRMCBSA-N

Formula:

C32H52O2

SMILES:

CC(=O)OC1CCC2(C)C(CC=C3C2CCC2(C)C3CCC2C(C)C2CC2(C)C(C)C(C)C)C1

Mol. weight [g/mol]:

468.75

Physical Properties

Property code	Value	Unit	Source
gf	193.59	kJ/mol	Joback Method
hf	-620.58	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.451		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	854.46	kPa	Joback Method
rinpol	3519.00		NIST Webbook
tb	1047.76	K	Joback Method
tc	1289.93	K	Joback Method
tf	617.68	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.23	J/mol×K	1047.76	Joback Method
cpg	1697.68	J/mol×K	1088.12	Joback Method
cpg	1745.89	J/mol×K	1128.48	Joback Method
cpg	1797.41	J/mol×K	1168.84	Joback Method
cpg	1852.81	J/mol×K	1209.20	Joback Method
cpg	1912.63	J/mol×K	1249.57	Joback Method
cpg	1977.43	J/mol×K	1289.93	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=R110960&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
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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