

Simiarenol (5-adianenol) acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C32H52O2/c1-20(2)22-10-13-25-29(22,6)16-18-32(9)26-14-11-23-24(30(26,7)

MBVFYSHTXNMYNB-DSSNUTGGSA-N

C32H52O2

CC(=O)OC1CCC2C(=CCC3C2(C)CCC2(C)C4CCC(C(C)C)C4(C)CCC32C)C1(C)C

468.75

Physical Properties

Property code	Value	Unit	Source
gf	167.68	kJ/mol	Joback Method
hf	-606.04	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3426.00		NIST Webbook
tb	1048.72	K	Joback Method
tc	1296.76	K	Joback Method
tf	687.72	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1688.55	J/molxK	1048.72	Joback Method
cpg	1749.18	J/molxK	1090.06	Joback Method
cpg	1815.48	J/molxK	1131.40	Joback Method
cpg	1888.28	J/molxK	1172.74	Joback Method
cpg	1968.41	J/molxK	1214.08	Joback Method
cpg	2056.69	J/molxK	1255.42	Joback Method
cpg	2153.95	J/molxK	1296.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R111438&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
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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