

Tetrahydrosmilagenin

Inchi:	InChI=1S/C27H48O3/c1-17(16-28)6-5-7-18(2)25-24(30)15-23-21-9-8-19-14-20(29)10-12
InchiKey:	QOZJGOAPWUNUFZ-UHFFFAOYSA-N
Formula:	C27H48O3
SMILES:	CC(CO)CCCC(C)C1C(O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	420.67

Physical Properties

Property code	Value	Unit	Source
gf	-105.91	kJ/mol	Joback Method
hf	-878.68	kJ/mol	Joback Method
hfus	45.70	kJ/mol	Joback Method
hvap	121.62	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.412		Crippen Method
mvol	365.460	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	1118.26	K	Joback Method
tc	1379.44	K	Joback Method
tf	627.27	K	Joback Method
vc	1.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1549.90	J/mol×K	1118.26	Joback Method
cpg	1591.52	J/mol×K	1161.79	Joback Method
cpg	1635.60	J/mol×K	1205.32	Joback Method
cpg	1682.65	J/mol×K	1248.85	Joback Method
cpg	1733.20	J/mol×K	1292.38	Joback Method
cpg	1787.75	J/mol×K	1335.91	Joback Method
cpg	1846.83	J/mol×K	1379.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U255290&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
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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