Neotigogenin

Inchi:	InChI=1S/C27H44O3/c1-16-7-12-27(29-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19(
InchiKey:	GMBQZIIUCVWOCD-ICOJOGTOSA-N
Formula:	C27H44O3
SMILES:	CC1CCC2(OC1)OC1CC3C4CCC5CC(O)CCC5(C)C4CCC3(C)C1C2C
Mol. weight [g/mol]:	416.64
CAS:	470-01-9

Physical Properties

Property code	Value	Unit	Source
gf	84.47	kJ/mol	Joback Method
hf	-699.48	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	96.77	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.794		Crippen Method
mcvol	343.740	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
tb	1006.27	K	Joback Method
tc	1247.23	K	Joback Method
tf	637.27	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1428.95	J/mol×K	1006.27	Joback Method
cpg	1469.35	J/mol×K	1046.43	Joback Method
cpg	1512.10	J/mol×K	1086.59	Joback Method
cpg	1557.75	J/mol×K	1126.75	Joback Method
cpg	1606.85	J/mol×K	1166.91	Joback Method
cpg	1659.94	J/mol×K	1207.07	Joback Method
cpg	1717.59	J/mol×K	1247.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C470019&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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