Solasodiene

Other names:	3,5-Solasodiene
	3,5-Solasodien, 3-dehydroxy-
	Solasodiene, 3-dehydroxy-
	3,5-Solasodine, 3-dehydroxy-
Inchi:	InChI=1S/C27H41NO/c1-17-10-14-27(28-16-17)18(2)24-23(29-27)15-22-20-9-8-19-7-5-6
InchiKey:	OYNIUJOJEWHJPN-UHFFFAOYSA-N
Formula:	C27H41NO
SMILES:	CC1CCC2(NC1)OC1CC3C4CC=C5C=CCCC5(C)C4CCC3(C)C1C2C
Mol. weight [g/mol]:	395.62
CAS:	3669-17-8

Physical Properties

Property code	Value	Unit	Source
gf	460.83	kJ/mol	Joback Method
hf	-232.67	kJ/mol	Joback Method
hfus	44.81	kJ/mol	Joback Method
hvap	84.20	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.092		Crippen Method
mcvol	333.380	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	3151.00		NIST Webbook
rinpol	3151.00		NIST Webbook
tb	948.33	K	Joback Method
tc	1207.00	K	Joback Method
tf	677.43	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.40	J/mol×K	948.33	Joback Method
cpg	1328.83	J/mol×K	991.44	Joback Method
cpg	1370.39	J/mol×K	1034.55	Joback Method

cpg	1414.76	J/mol×K	1077.67	Joback Method
cpg	1462.61	J/mol×K	1120.78	Joback Method
cpg	1514.65	J/mol×K	1163.89	Joback Method
cpg	1571.54	J/mol×K	1207.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3669178&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