

Solasodine

Other names:

Spirosol-5-en-3-ol, (3«beta»,22«alpha»,25R)-
Solasod-5-en-3«beta»-ol
Purapuridine
Salasdine
Salasodine
Solancarpidine
Solanidine-S
Solasodin
Spiro[8H-naphth[2',1':4,5]indeno[2,1-b]furan-8,2'-piperidine], spirosol-5-en-3-ol
deriv
NSC 178260
NSC 179187
Solasod-5-en-3-beta-ol

Inchi: InChI=1S/C27H43NO2/c1-16-7-12-27(28-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19**InchiKey:** KWVISVAMQJWJSZ-ICPPQKBESA-N**Formula:** C27H43NO2**SMILES:** CC1CCC2(NC1)OC1CC3C4CC=C5CC(O)CCC5(C)C4CCC3(C)C1C2C**Mol. weight [g/mol]:** 413.64**CAS:** 126-17-0

Physical Properties

Property code	Value	Unit	Source
gf	286.34	kJ/mol	Joback Method
hf	-463.02	kJ/mol	Joback Method
hfus	48.75	kJ/mol	Joback Method
hvap	100.28	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.287		Crippen Method
mcvol	343.550	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	3338.00		NIST Webbook
tb	1036.68	K	Joback Method
tc	1283.82	K	Joback Method
tf	733.25	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1429.80	J/molxK	1036.68	Joback Method
cpg	1472.83	J/molxK	1077.87	Joback Method
cpg	1518.85	J/molxK	1119.06	Joback Method
cpg	1568.43	J/molxK	1160.25	Joback Method
cpg	1622.17	J/molxK	1201.44	Joback Method
cpg	1680.66	J/molxK	1242.63	Joback Method
cpg	1744.46	J/molxK	1283.82	Joback Method

Sources

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=C126170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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