Cholestan-3-one, (5«beta»)-

Other names:	Coprostan-3-one
	5«beta»-Cholestan-3-one
	Coprostanone
	5B-Cholestan-3-one
Inchi:	InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
InchiKey:	PESKGJQREUXSRR-GPWPMFNDSA-N
Formula:	C27H46O
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	386.65
CAS:	601-53-6

Physical Properties

Property code	Value	Unit	Source
gf	197.38	kJ/mol	Joback Method
hf	-519.01	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.677		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3057.00		NIST Webbook
tb	918.88	K	Joback Method
tc	1150.52	K	Joback Method
tf	521.51	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.06	J/mol×K	918.88	Joback Method
cpg	1339.92	J/mol×K	957.49	Joback Method
cpg	1371.74	J/mol×K	996.09	Joback Method

cpg	1403.86	J/mol×K	1034.70	Joback Method
cpg	1436.61	J/mol×K	1073.31	Joback Method
cpg	1470.31	J/mol×K	1111.92	Joback Method
cpg	1505.29	J/mol×K	1150.52	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=C601536&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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