Cholestane

Other names:	Cholestane, (5«alpha»)- 5«alpha»-Cholestane «alpha»-Cholestane 28,29,30-Trinorlanostane 10,13-Dimethyl-17-(1',5'-dimethylhexyl)-hexadecahydrocyclopenta(a)phenanthrene 5A-Cholestane, TMS 17-(1,5-Dimethylhexyl)-10,13-dimethyl-hexahydro-1H-cyclopenta[a]-phenanthrene (5-«alpha»-cholestane)
Inchi:	InChI=1S/C27H48/c1-19(2)9-8-10-20(3)23-14-15-24-22-13-12-21-11-6-7-17-26(21,4)25(
InchiKey:	XIIAYQZJNBULGD-BTSBFKJRSA-N
Formula:	C27H48
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]:	372.67
CAS:	481-21-0

Physical Properties

Property code	Value	Unit	Source
gf	319.97	kJ/mol	Joback Method
hf	-381.31	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hsub	133.80	kJ/mol	NIST Webbook
hvap	72.20	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.498		Crippen Method
mcvol	347.850	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2819.00		NIST Webbook
rinpol	2838.00		NIST Webbook
rinpol	2856.00		NIST Webbook
rinpol	2852.00		NIST Webbook
rinpol	2866.00		NIST Webbook
rinpol	2856.00		NIST Webbook
rinpol	2852.00		NIST Webbook
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
rinpol	2866.00		NIST Webbook
tb	851.06	K	Joback Method

tc	1072.72	K	Joback Method
tf	453.29	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.75	J/mol×K	851.06	Joback Method
cpg	1282.08	J/mol×K	888.00	Joback Method
cpg	1312.99	J/mol×K	924.95	Joback Method
cpg	1343.81	J/mol×K	961.89	Joback Method
cpg	1374.86	J/mol×K	998.83	Joback Method
cpg	1406.45	J/mol×K	1035.78	Joback Method
cpg	1438.92	J/mol×K	1072.72	Joback Method
hfust	25.40	kJ/mol	351.80	NIST Webbook
hvapt	108.40	kJ/mol	352.00	NIST Webbook
hvapt	115.60	kJ/mol	509.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C481210&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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
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