

1H-Cyclopenta[a]phenanthrene, 17-(1,5-dimethylhexyl)hexadecahydro-4,4,10,13,14-oxo- [5S-[5«alpha»,8«beta»,9«alpha»,10«beta»,13«beta»

Other names: Lanostane
Cholestane, 4,4,14-trimethyl-, (5«alpha»)-

Inchi: InChI=1S/C30H54/c1-21(2)11-9-12-22(3)23-15-19-30(8)25-13-14-26-27(4,5)17-10-18-28

InchiKey: ZQIOPEXWVBIZAV-UHFFFAOYSA-N

Formula: C30H54

SMILES: CC(C)CCCC(C)C1CCC2(C)C3CCC4C(C)(C)CCCC4(C)C3CCC12C

Mol. weight [g/mol]: 414.75

CAS: 474-20-4

Physical Properties

Property code	Value	Unit	Source
gf	326.54	kJ/mol	Joback Method
hf	-433.09	kJ/mol	Joback Method
hfus	27.54	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	9.524		Crippen Method
mcvol	390.120	ml/mol	McGowan Method
pc	870.68	kPa	Joback Method
rinpol	3027.00		NIST Webbook
rinpol	3027.00		NIST Webbook
tb	915.51	K	Joback Method
tc	1142.56	K	Joback Method
tf	530.66	K	Joback Method
vc	1.480	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1459.47	J/molxK	915.51	Joback Method
cpg	1499.78	J/molxK	953.35	Joback Method
cpg	1541.84	J/molxK	991.19	Joback Method

cpg	1586.18	J/mol×K	1029.03	Joback Method
cpg	1633.35	J/mol×K	1066.88	Joback Method
cpg	1683.90	J/mol×K	1104.72	Joback Method
cpg	1738.37	J/mol×K	1142.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C474204&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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