

Cholestan-3«alpha»-ol acetate

Other names:	Epicholestanol acetate
Inchi:	InChI=1S/C29H50O2/c1-19(2)8-7-9-20(3)25-12-13-26-24-11-10-22-18-23(31-21(4)30)14
InchiKey:	PHLIUSDPFOUISN-UHFFFAOYSA-N
Formula:	C29H50O2
SMILES:	CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	430.71

Physical Properties

Property code	Value	Unit	Source
hfus	40.34	kJ/mol	Joback Method
hvap	131.22	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.77		Cheméo Relay (1.0)
logp	8.039		Crippen Method
mcvol	383.470	ml/mol	McGowan Method
rinpol	3151.00		NIST Webbook
rinpol	3151.00		NIST Webbook
tb	691.20	K	Cheméo Relay (1.0)
tf	385.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.89	J/mol×K	968.44	Joback Method
cpg	1498.65	J/mol×K	1006.28	Joback Method
cpg	1531.69	J/mol×K	1044.12	Joback Method
cpg	1565.33	J/mol×K	1081.96	Joback Method
cpg	1599.90	J/mol×K	1119.80	Joback Method
cpg	1635.71	J/mol×K	1157.64	Joback Method
cpg	1673.10	J/mol×K	1195.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U214832&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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