24-Ethyl-5-«alpha»-cholest-8-en-3-«beta»-ol

Inchi: InChI=1S/C29H50O/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(30)14-16-2
InchiKey: YCBMXIIYHMNHDU-RUVYBSODSA-N
Formula: C29H50O
SMILES: CCC(CCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1CC3)C(C)C
Mol. weight [g/mol]: 414.71

Physical Properties

Property code	Value	Unit	Source
gf	215.96	kJ/mol	Joback Method
hf	-524.92	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	94.87	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	8.169		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook
tb	1002.35	K	Joback Method
tc	1229.83	K	Joback Method
tf	551.69	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1456.25	J/mol×K	1002.35	Joback Method
cpg	1489.75	J/mol×K	1040.26	Joback Method
cpg	1524.21	J/mol×K	1078.18	Joback Method
cpg	1559.99	J/mol×K	1116.09	Joback Method
cpg	1597.42	J/mol×K	1154.00	Joback Method
cpg	1636.88	J/mol×K	1191.91	Joback Method
cpg	1678.71	J/mol×K	1229.83	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=R214676&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