

5-«beta»-cholestan-3«alpha»-ol, butyrate

Inchi:	InChI=1S/C31H54O2/c1-7-9-29(32)33-24-16-18-30(5)23(20-24)12-13-25-27-15-14-26(22)
InchiKey:	QFYCBKBNZGFRP-UHFFFAOYSA-N
Formula:	C31H54O2
SMILES:	CCCC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	458.76

Physical Properties

Property code	Value	Unit	Source
gf	112.02	kJ/mol	Joback Method
hf	-729.01	kJ/mol	Joback Method
hfus	45.51	kJ/mol	Joback Method
hvap	89.95	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.820		Crippen Method
mcvol	411.650	ml/mol	McGowan Method
pc	802.97	kPa	Joback Method
rinpol	2809.00		NIST Webbook
tb	1014.20	K	Joback Method
tc	1244.64	K	Joback Method
tf	566.29	K	Joback Method
vc	1.563	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1609.33	J/mol×K	1014.20	Joback Method
cpg	1644.56	J/mol×K	1052.61	Joback Method
cpg	1680.38	J/mol×K	1091.01	Joback Method
cpg	1717.14	J/mol×K	1129.42	Joback Method
cpg	1755.20	J/mol×K	1167.83	Joback Method
cpg	1794.89	J/mol×K	1206.24	Joback Method
cpg	1836.56	J/mol×K	1244.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368377&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

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
mccvol:	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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