

Cholesteryl butyrate

Other names:	5-Cholesten-3«beta»-ol butyrate Cholesterol n-butyrate Cholest-5-en-3-ol (3«beta»)-, butanoate 3«beta»-Butanoyloxycholest-5-ene cholest-5-en-3«beta»-ol butyrate
Inchi:	InChI=1S/C31H52O2/c1-7-9-29(32)33-24-16-18-30(5)23(20-24)12-13-25-27-15-14-26(22)
InchiKey:	CKDZWMVGDHGMFR-UHFFFAOYSA-N
Formula:	C31H52O2
SMILES:	CCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	456.74
CAS:	521-13-1

Physical Properties

Property code	Value	Unit	Source
gf	140.06	kJ/mol	Joback Method
hf	-662.36	kJ/mol	Joback Method
hfus	45.28	kJ/mol	Joback Method
hvap	91.22	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.740		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	828.11	kPa	Joback Method
tb	1023.01	K	Joback Method
tc	1255.41	K	Joback Method
tf	583.81	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1575.99	J/molxK	1023.01	Joback Method
cpg	1611.10	J/molxK	1061.74	Joback Method
cpg	1647.03	J/molxK	1100.48	Joback Method
cpg	1684.16	J/molxK	1139.21	Joback Method

cpg	1722.84	J/mol×K	1177.95	Joback Method
cpg	1763.43	J/mol×K	1216.68	Joback Method
cpg	1806.30	J/mol×K	1255.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C521131&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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