

Cholesteryl caprate

Other names:

Cholesteryl decanoate
5-Cholesten-3«beta»-ol decylate
Cholest-5-en-3-ol (3«beta»)-, decanoate
3«beta»-Decanoyloxycholest-5-ene
cholest-5-en-3-«beta»-yl decanoate
(3«beta»)-cholest-5-3-yl decanoate

Inchi:

InChI=1S/C37H64O2/c1-7-8-9-10-11-12-13-17-35(38)39-30-22-24-36(5)29(26-30)18-19-

InchiKey:

LJGMGXCKVFFIS-ZOFIJQIFSA-N

Formula:

C37H64O2

SMILES:

CCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1

Mol. weight [g/mol]:

540.90

CAS:

1183-04-6

Physical Properties

Property code	Value	Unit	Source
gf	190.58	kJ/mol	Joback Method
hf	-786.20	kJ/mol	Joback Method
hfus	60.82	kJ/mol	Joback Method
hvap	104.57	kJ/mol	Joback Method
log10ws	-11.78		Crippen Method
logp	11.080		Crippen Method
mcvol	491.890	ml/mol	McGowan Method
pc	609.36	kPa	Joback Method
tb	1160.29	K	Joback Method
tc	1428.97	K	Joback Method
tf	651.43	K	Joback Method
vc	1.887	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2033.01	J/mol×K	1160.29	Joback Method
cpg	2083.43	J/mol×K	1205.07	Joback Method
cpg	2136.47	J/mol×K	1249.85	Joback Method

cpg	2192.72	J/mol×K	1294.63	Joback Method
cpg	2252.78	J/mol×K	1339.41	Joback Method
cpg	2317.23	J/mol×K	1384.19	Joback Method
cpg	2386.68	J/mol×K	1428.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1183046&Units=SI
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

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

Latest version available from:

<https://www.chemeo.com/cid/73-462-8/Cholesteryl-caprate.pdf>

Generated by Cheméo on 2024-04-28 00:19:30.888694802 +0000 UTC m=+16552819.809272114.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.