5-Oxo-3,5-seco-a-norcholestan-3-oic acid

Inchi: InChI=1S/C26H44O3/c1-17(2)7-6-8-18(3)20-10-11-21-19-9-12-23(27)26(5,16-14-24(28)2
InchiKey: YSWDCQJTPYALJE-UHFFFAOYSA-N
Formula: C26H44O3
SMILES: CC(C)CCCC(C)C1CCC2C3CCC(=O)C(C)(CCC(=O)O)C3CCC12C
Mol. weight [g/mol]: 404.63
CAS: 1508-94-7

Physical Properties

Property code	Value	Unit	Source
gf	-125.43	kJ/mol	Joback Method
hf	-829.82	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	97.56	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.741		Crippen Method
mcvol	353.630	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
tb	1031.04	K	Joback Method
tc	1263.41	K	Joback Method
tf	606.57	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1374.14	J/mol×K	1031.04	Joback Method
cpg	1405.29	J/mol×K	1069.77	Joback Method
cpg	1437.23	J/mol×K	1108.50	Joback Method
cpg	1470.29	J/mol×K	1147.22	Joback Method
cpg	1504.77	J/mol×K	1185.95	Joback Method
cpg	1540.96	J/mol×K	1224.68	Joback Method
cpg	1579.18	J/mol×K	1263.41	Joback Method

Sources

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=C1508947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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