

16Beta-carboxy-17alpha-pregn-5-en-3beta-ol-20-o

Inchi:	InChI=1S/C24H34O5/c1-13(25)21-18(22(27)28)12-20-17-6-5-15-11-16(29-14(2)26)7-9-2
InchiKey:	VCRJNQOFXWUBMO-UHFFFAOYSA-N
Formula:	C24H34O5
SMILES:	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C3CC(C(=O)O)C2C(C)=O)C1
Mol. weight [g/mol]:	402.52
CAS:	1434-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-316.37	kJ/mol	Joback Method
hf	-905.05	kJ/mol	Joback Method
hfus	42.55	kJ/mol	Joback Method
hvap	106.27	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.397		Crippen Method
mcvol	317.730	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
tb	1058.98	K	Joback Method
tc	1300.02	K	Joback Method
tf	691.36	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.26	J/molxK	1058.98	Joback Method
cpg	1269.65	J/molxK	1099.15	Joback Method
cpg	1301.49	J/molxK	1139.33	Joback Method
cpg	1335.15	J/molxK	1179.50	Joback Method
cpg	1370.97	J/molxK	1219.67	Joback Method
cpg	1409.31	J/molxK	1259.85	Joback Method
cpg	1450.53	J/molxK	1300.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1434624&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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