5-Pregnen-3«beta»-ol-20-one, butyrate

Inchi: InChI=1S/C25H38O3/c1-5-6-23(27)28-18-11-13-24(3)17(15-18)7-8-19-21-10-9-20(16(2)2
InchiKey: DTHSTPZCWGYBFE-UHFFFAOYSA-N
Formula: C25H38O3
SMILES: CCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC32)C1
Mol. weight [g/mol]: 386.57

Physical Properties

Property code	Value	Unit	Source
gf	-34.50	kJ/mol	Joback Method
hf	-640.54	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	85.38	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.866		Crippen Method
mcvol	324.380	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2546.00		NIST Webbook
tb	940.48	K	Joback Method
tc	1173.36	K	Joback Method
tf	596.12	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.78	J/mol×K	940.48	Joback Method
cpg	1218.37	J/mol×K	979.29	Joback Method
cpg	1247.39	J/mol×K	1018.11	Joback Method
cpg	1277.17	J/mol×K	1056.92	Joback Method
cpg	1308.04	J/mol×K	1095.73	Joback Method
cpg	1340.33	J/mol×K	1134.54	Joback Method
cpg	1374.39	J/mol×K	1173.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368372&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
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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