

Trans-androsterone, butyrate

Inchi: InChI=1S/C23H36O3/c1-4-5-21(25)26-16-10-12-22(2)15(14-16)6-7-17-18-8-9-20(24)23(2)
InchiKey: ZBPQBCXWLUSWGS-UHFFFAOYSA-N
Formula: C23H36O3
SMILES: CCCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 360.53

Physical Properties

Property code	Value	Unit	Source
gf	-65.34	kJ/mol	Joback Method
hf	-670.69	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	77.48	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.310		Crippen Method
mvol	300.500	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	904.53	K	Joback Method
tc	1143.14	K	Joback Method
tf	578.59	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.74	J/molxK	904.53	Joback Method
cpg	1135.18	J/molxK	944.30	Joback Method
cpg	1163.60	J/molxK	984.07	Joback Method
cpg	1192.31	J/molxK	1023.83	Joback Method
cpg	1221.63	J/molxK	1063.60	Joback Method
cpg	1251.89	J/molxK	1103.37	Joback Method
cpg	1283.39	J/molxK	1143.14	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=U368382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/88-722-3/Trans-androsterone-butyrate.pdf>

Generated by Cheméo on 2024-04-23 10:40:48.497569823 +0000 UTC m=+16158097.418147135.

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