

Trans-androsterone, 4-chlorobutyrate

Inchi: InChI=1S/C23H35ClO3/c1-22-11-9-16(27-21(26)4-3-13-24)14-15(22)5-6-17-18-7-8-20(23)/h1-10,12-15,17-20,22-24,26-27/t16,21
InchiKey: CXIUHMPDEUPPPV-UHFFFAOYSA-N
Formula: C23H35ClO3
SMILES: CC12CCC3C(CCC4CC(OC(=O)CCCCl)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 394.98

Physical Properties

Property code	Value	Unit	Source
gf	-77.27	kJ/mol	Joback Method
hf	-686.43	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	81.86	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.529		Crippen Method
mcvol	312.740	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2673.00		NIST Webbook
rinpol	2673.00		NIST Webbook
tb	941.96	K	Joback Method
tc	1183.48	K	Joback Method
tf	608.51	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.21	J/mol×K	941.96	Joback Method
cpg	1170.67	J/mol×K	982.21	Joback Method
cpg	1199.43	J/mol×K	1022.47	Joback Method
cpg	1228.83	J/mol×K	1062.72	Joback Method
cpg	1259.21	J/mol×K	1102.97	Joback Method
cpg	1290.88	J/mol×K	1143.22	Joback Method
cpg	1324.20	J/mol×K	1183.48	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368384&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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