3-Oxoandrost-4-ene-17B-carboxaldehyde

Inchi: InChI=1S/C20H28O2/c1-19-9-7-15(22)11-13(19)3-5-16-17-6-4-14(12-21)20(17,2)10-8-18
InchiKey: VZHQDHQAMFXIJW-JQBYYDJRSA-N
Formula: C20H28O2
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C(C=O)CCC12
Mol. weight [g/mol]: 300.44

Physical Properties

Property code	Value	Unit	Source
gf	71.84	kJ/mol	Joback Method
hf	-382.90	kJ/mol	Joback Method
hfus	21.77	kJ/mol	Joback Method
hvap	69.63	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.333		Crippen Method
mcvol	248.060	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	817.07	K	Joback Method
tc	1068.50	K	Joback Method
tf	532.14	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.60	J/mol×K	817.07	Joback Method
cpg	875.39	J/mol×K	858.98	Joback Method
cpg	900.93	J/mol×K	900.88	Joback Method
cpg	926.59	J/mol×K	942.79	Joback Method
cpg	952.77	J/mol×K	984.69	Joback Method
cpg	979.86	J/mol×K	1026.60	Joback Method
cpg	1008.24	J/mol×K	1068.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R93042&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