

2-Oxa-5beta-androstan-3-one, 4beta,5-epoxy-17beta-hydroxy-

Inchi:	InChI=1S/C18H26O4/c1-16-7-6-12-10(11(16)3-4-13(16)19)5-8-18-14(22-18)15(20)21-9-
InchiKey:	MDIANPPZAJCEKU-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CC12CCC3C(CCC45OC4C(=O)OCC35C)C1CCC2O
Mol. weight [g/mol]:	306.40
CAS:	4354-23-8

Physical Properties

Property code	Value	Unit	Source
gf	-103.12	kJ/mol	Joback Method
hf	-638.56	kJ/mol	Joback Method
hfus	30.63	kJ/mol	Joback Method
hvap	81.31	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.284		Crippen Method
mcvol	229.360	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	858.36	K	Joback Method
tc	1098.72	K	Joback Method
tf	612.92	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.95	J/molxK	858.36	Joback Method
cpg	878.70	J/molxK	898.42	Joback Method
cpg	905.71	J/molxK	938.48	Joback Method
cpg	934.49	J/molxK	978.54	Joback Method
cpg	965.52	J/molxK	1018.60	Joback Method
cpg	999.32	J/molxK	1058.66	Joback Method
cpg	1036.38	J/molxK	1098.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4354238&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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