10Beta-fluoro-17beta-hydroxy-estra-1,4-dien-3-on

Inchi: InChI=1S/C18H23FO2/c1-17-8-7-15-13(14(17)4-5-16(17)21)3-2-11-10-12(20)6-9-18(11,1
InchiKey: KMESAHJOIFFQAU-UHFFFAOYSA-N
Formula: C18H23FO2
SMILES: CC12CCC3C(CCC4=CC(=O)C=CC43F)C1CCC2O
Mol. weight [g/mol]: 290.37
CAS: 1427-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-147.15	kJ/mol	Joback Method
hf	-546.60	kJ/mol	Joback Method
hfus	22.70	kJ/mol	Joback Method
hvap	74.61	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.357		Crippen Method
mcvol	221.650	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
tb	813.26	K	Joback Method
tc	1046.23	K	Joback Method
tf	529.77	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.38	J/mol×K	813.26	Joback Method
cpg	779.75	J/mol×K	852.09	Joback Method
cpg	801.04	J/mol×K	890.92	Joback Method
cpg	822.55	J/mol×K	929.74	Joback Method
cpg	844.59	J/mol×K	968.57	Joback Method
cpg	867.46	J/mol×K	1007.40	Joback Method
cpg	891.47	J/mol×K	1046.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1427618&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume