

5Alpha-androstane, 3,3,17,17-tetrafluoro-

Inchi:	InChI=1S/C19H28F4/c1-16-9-10-18(20,21)11-12(16)3-4-13-14(16)5-7-17(2)15(13)6-8-19
InchiKey:	QXAFOMSOCXJHRA-UHFFFAOYSA-N
Formula:	C19H28F4
SMILES:	CC12CCC(F)(F)CC1CCC1C2CCC2(C)C1CCC2(F)F
Mol. weight [g/mol]:	332.42
CAS:	3834-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-540.44	kJ/mol	Joback Method
hf	-979.93	kJ/mol	Joback Method
hfus	18.42	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.300		Crippen Method
mvol	242.210	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
tb	661.79	K	Joback Method
tc	879.88	K	Joback Method
tf	439.05	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/molxK	661.79	Joback Method
cpg	793.54	J/molxK	698.14	Joback Method
cpg	818.14	J/molxK	734.49	Joback Method
cpg	842.25	J/molxK	770.83	Joback Method
cpg	866.32	J/molxK	807.18	Joback Method
cpg	890.79	J/molxK	843.53	Joback Method
cpg	916.13	J/molxK	879.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3834182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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