

Estradiol, HFB

Inchi:	InChI=1S/C26H22F14O4/c1-20-9-8-14-13-5-3-12(43-18(41)21(27,28)23(31,32)25(35,36)
InchiKey:	NPCTWMQURTYGTA-HSQSFYGFSA-N
Formula:	C26H22F14O4
SMILES:	CC12CCC3c4ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	664.43

Physical Properties

Property code	Value	Unit	Source
gf	-2779.81	kJ/mol	Joback Method
hf	-3473.38	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.026		Crippen Method
mvol	360.520	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	973.56	K	Joback Method
tc	1192.35	K	Joback Method
tf	663.54	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.23	J/molxK	973.56	Joback Method
cpg	1327.73	J/molxK	1010.02	Joback Method
cpg	1347.67	J/molxK	1046.49	Joback Method
cpg	1368.37	J/molxK	1082.95	Joback Method
cpg	1390.17	J/molxK	1119.42	Joback Method
cpg	1413.39	J/molxK	1155.88	Joback Method
cpg	1438.37	J/molxK	1192.35	Joback Method

Sources

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=R169927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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