Estrone, heptafluorobutyrate

Other names: 17-Oxoestra-1,3,5(10)-trien-3-yl 2,2,3,3,4,4,4-heptafluorobutanoate
Inchi: InChI=1S/C22H21F7O3/c1-19-9-8-14-13-5-3-12(32-18(31)20(23,24)21(25,26)22(27,28)2
InchiKey: VPKYJRGMBQKKDH-UHFFFAOYSA-N
Formula: C22H21F7O3
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc4CCC3C1CCC2=O
Mol. weight [g/mol]: 466.39
CAS: 2192-60-1

Physical Properties

Property code	Value	Unit	Source
gf	-1339.30	kJ/mol	Joback Method
hf	-1864.36	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	5.850		Crippen Method
mcvol	285.900	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2495.20		NIST Webbook
rinpol	2495.20		NIST Webbook
tb	893.04	K	Joback Method
tc	1112.65	K	Joback Method
tf	607.37	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.49	J/mol×K	893.04	Joback Method
cpg	1012.67	J/mol×K	929.64	Joback Method
cpg	1030.57	J/mol×K	966.24	Joback Method
cpg	1048.42	J/mol×K	1002.85	Joback Method
cpg	1066.47	J/mol×K	1039.45	Joback Method
cpg	1084.94	J/mol×K	1076.05	Joback Method

cpg	1104.09	J/mol×K	1112.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2192601&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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