16-Epiestriol, tris(pentafluoropropionate)

Inchi: InChI=1S/C27H21F15O6/c1-21-7-6-13-12-5-3-11(46-18(43)22(28,29)25(34,35)36)8-10(1
InchiKey: WNINQNBIZUYHQT-UHFFFAOYSA-N
Formula: C27H21F15O6
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)C(F)(F)F)cc4CCC3C1CC(OC(=O)C(F)(F)C(F)(F)F)C2C
Mol. weight [g/mol]: 726.43

Physical Properties

Property code	Value	Unit	Source
gf	-3207.83	kJ/mol	Joback Method
hf	-3955.27	kJ/mol	Joback Method
hfus	56.15	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	7.474		Crippen Method
mcvol	383.820	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	2454.60		NIST Webbook
rinpol	2454.60		NIST Webbook
tb	1067.33	K	Joback Method
tc	1318.48	K	Joback Method
tf	743.32	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1431.31	J/mol×K	1067.33	Joback Method
cpg	1454.72	J/mol×K	1109.19	Joback Method
cpg	1479.42	J/mol×K	1151.05	Joback Method
cpg	1505.87	J/mol×K	1192.91	Joback Method
cpg	1534.53	J/mol×K	1234.77	Joback Method
cpg	1565.89	J/mol×K	1276.62	Joback Method
cpg	1600.40	J/mol×K	1318.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352394&Units=SI

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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