Ethinylestradiol, HFB

Inchi: InChI=1S/C28H22F14O4/c1-3-22(46-20(44)24(31,32)26(35,36)28(40,41)42)11-9-18-17-6
InchiKey: JXDGOQVCSYQGEA-VUTDOMMHSA-N
Formula: C28H22F14O4
SMILES: C#CC1(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC2C3CCc4cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 688.45

Physical Properties

Property code	Value	Unit	Source
gf	-2545.39	kJ/mol	Joback Method
hf	-3207.52	kJ/mol	Joback Method
hfus	48.48	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.029		Crippen Method
mcvol	380.100	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	1009.68	K	Joback Method
tc	1236.43	K	Joback Method
tf	756.95	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.71	J/mol×K	1009.68	Joback Method
cpg	1408.30	J/mol×K	1047.47	Joback Method
cpg	1436.96	J/mol×K	1085.26	Joback Method
cpg	1468.16	J/mol×K	1123.05	Joback Method
cpg	1502.38	J/mol×K	1160.85	Joback Method
cpg	1540.10	J/mol×K	1198.64	Joback Method
cpg	1581.79	J/mol×K	1236.43	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=R169947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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