Stigmastanol, pentafluoropropionate

Inchi: InChI=1S/C32H51F5O2/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(39-28(
InchiKey: DSZLEQOIFPKYAL-UHFFFAOYSA-N
Formula: C32H51F5O2
SMILES: CCC(CCC(C)C1CCC2C3CCC4CC(OC(=O)C(F)(F)C(F)(F)F)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 562.74

Physical Properties

Property code	Value	Unit	Source
gf	-850.37	kJ/mol	Joback Method
hf	-1752.98	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	9.853		Crippen Method
mcvol	434.590	ml/mol	McGowan Method
pc	691.07	kPa	Joback Method
rinpol	3158.50		NIST Webbook
rinpol	3158.50		NIST Webbook
tb	1026.53	K	Joback Method
tc	1256.78	K	Joback Method
tf	570.35	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1710.92	J/mol×K	1026.53	Joback Method
cpg	1746.35	J/mol×K	1064.90	Joback Method
cpg	1782.78	J/mol×K	1103.28	Joback Method
cpg	1820.63	J/mol×K	1141.65	Joback Method
cpg	1860.30	J/mol×K	1180.03	Joback Method
cpg	1902.20	J/mol×K	1218.40	Joback Method
cpg	1946.74	J/mol×K	1256.78	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=U352392&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