

Corticosterone, bis(pentafluoropropionate)

Inchi:	InChI=1S/C27H28F10O6/c1-22-8-7-13(38)9-12(22)3-4-14-15-5-6-16(17(39)11-42-20(40)
InchiKey:	NCDGBEXLHJZLSR-UHFFFAOYSA-N
Formula:	C27H28F10O6
SMILES:	CC12CCC(=O)C=C1CCC1C2C(OC(=O)C(F)(F)C(F)(F)F)CC2(C)C(C(=O)COC(=O)C(F)(
Mol. weight [g/mol]:	638.49

Physical Properties

Property code	Value	Unit	Source
gf	-2310.91	kJ/mol	Joback Method
hf	-3060.42	kJ/mol	Joback Method
hfus	47.00	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.164		Crippen Method
mcvol	379.270	ml/mol	McGowan Method
pc	898.02	kPa	Joback Method
rinpola	2918.80		NIST Webbook
rinpola	2918.80		NIST Webbook
tb	1110.13	K	Joback Method
tc	1361.82	K	Joback Method
tf	774.62	K	Joback Method
vc	1.512	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1500.90	J/molxK	1110.13	Joback Method
cpg	1534.73	J/molxK	1152.08	Joback Method
cpg	1571.05	J/molxK	1194.03	Joback Method
cpg	1610.35	J/molxK	1235.97	Joback Method
cpg	1653.16	J/molxK	1277.92	Joback Method
cpg	1699.97	J/molxK	1319.87	Joback Method
cpg	1751.29	J/molxK	1361.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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