

Pregnanediol, TFA

Other names:	5-«beta»-Pregnan-3-«alpha»,20-«beta»-diol, TFA
Inchi:	InChI=1S/C25H34F6O4/c1-13(34-20(32)24(26,27)28)17-6-7-18-16-5-4-14-12-15(35-21(3
InchiKey:	ZYWWYWQPOLCWDY-ULRPYYSESA-N
Formula:	C25H34F6O4
SMILES:	CC(OC(=O)C(F)(F)F)C1CCC2C3CCC4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	512.53

Physical Properties

Property code	Value	Unit	Source
gf	-1333.16	kJ/mol	Joback Method
hf	-2038.85	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.613		Crippen Method
mcvol	345.170	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
rinpol	2462.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	942.81	K	Joback Method
tc	1159.83	K	Joback Method
tf	594.21	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.92	J/molxK	942.81	Joback Method
cpg	1323.94	J/molxK	978.98	Joback Method
cpg	1350.26	J/molxK	1015.15	Joback Method
cpg	1377.20	J/molxK	1051.32	Joback Method
cpg	1405.06	J/molxK	1087.49	Joback Method

cpg	1434.12	J/mol×K	1123.66	Joback Method
cpg	1464.71	J/mol×K	1159.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R305341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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