

16«alpha»-Methylpregnenolone, TFA

Inchi: InChI=1S/C24H33F3O3/c1-13-11-19-17-6-5-15-12-16(30-21(29)24(25,26)27)7-9-22(15,30)
InchiKey: QUUCZLZUBSTNFM-FIVICNPVSA-N
Formula: C24H33F3O3
SMILES: CC(=O)C1C(C)CC2C3CC=C4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 426.51

Physical Properties

Property code	Value	Unit	Source
gf	-632.22	kJ/mol	Joback Method
hf	-1237.32	kJ/mol	Joback Method
hfus	38.69	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.875		Crippen Method
mcvol	315.600	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	907.51	K	Joback Method
tc	1130.72	K	Joback Method
tf	584.80	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.99	J/mol×K	907.51	Joback Method
cpg	1172.77	J/mol×K	944.71	Joback Method
cpg	1198.74	J/mol×K	981.91	Joback Method
cpg	1225.21	J/mol×K	1019.11	Joback Method
cpg	1252.49	J/mol×K	1056.31	Joback Method
cpg	1280.88	J/mol×K	1093.52	Joback Method
cpg	1310.70	J/mol×K	1130.72	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=R305138&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
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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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