

Tofisopam

Other names:	5H-2,3-Benzodiazepine, 1-(3,4-dimethoxyphenyl)-5-ethyl-7,8-dimethoxy-4-methyl-1-(3,4-Dimethoxyphenyl)-5-ethyl-7,8-dimethoxy-4-methyl-5H-2,3-benzodiazepine Egyt 341 Grandaxin TF Seriel
Inchi:	InChI=1S/C22H26N2O4/c1-7-15-13(2)23-24-22(14-8-9-18(25-3)19(10-14)26-4)17-12-21
InchiKey:	RUJBDQSFYCKFAA-UHFFFAOYSA-N
Formula:	C22H26N2O4
SMILES:	<chem>CCC1C(C)=NN=C(c2ccc(OC)c(OC)c2)c2cc(OC)c(OC)cc21</chem>
Mol. weight [g/mol]:	382.45
CAS:	22345-47-7

Physical Properties

Property code	Value	Unit	Source
gf	201.80	kJ/mol	Joback Method
hf	-315.54	kJ/mol	Joback Method
hfus	49.50	kJ/mol	Joback Method
hvap	96.65	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.441		Crippen Method
mcvol	297.300	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	3055.00		NIST Webbook
tb	1001.66	K	Joback Method
tc	1245.75	K	Joback Method
tf	722.60	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.48	J/molxK	1001.66	Joback Method
cpg	1011.63	J/molxK	1042.34	Joback Method

cpg	1020.15	J/mol×K	1083.02	Joback Method
cpg	1025.98	J/mol×K	1123.71	Joback Method
cpg	1029.06	J/mol×K	1164.39	Joback Method
cpg	1029.31	J/mol×K	1205.07	Joback Method
cpg	1026.67	J/mol×K	1245.75	Joback Method

Sources

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=C22345477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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