

Teferin

Inchi:	InChI=1S/C23H32O5/c1-14(2)23(26)11-10-22(4)9-8-15(3)12-19(20(22)23)28-21(25)16-6
InchiKey:	YEQVRBJRNFLOQJ-KKSHJYNMSA-N
Formula:	C23H32O5
SMILES:	<chem>COc1cc(C(=O)OC2CC(C)=CCC3(C)CCC(O)(C(C)C)C23)ccc1O</chem>
Mol. weight [g/mol]:	388.50

Physical Properties

Property code	Value	Unit	Source
gf	-320.21	kJ/mol	Joback Method
hf	-847.76	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	109.15	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.470		Crippen Method
mvol	310.200	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	1054.21	K	Joback Method
tc	1296.97	K	Joback Method
tf	714.24	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.23	J/mol×K	1054.21	Joback Method
cpg	1180.19	J/mol×K	1094.67	Joback Method
cpg	1211.90	J/mol×K	1135.13	Joback Method
cpg	1245.72	J/mol×K	1175.59	Joback Method
cpg	1281.99	J/mol×K	1216.05	Joback Method
cpg	1321.06	J/mol×K	1256.51	Joback Method
cpg	1363.30	J/mol×K	1296.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200305&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
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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