Teferidine

Inchi: InChI=1S/C22H30O3/c1-15(2)22(24)13-12-21(4)11-10-16(3)14-18(19(21)22)25-20(23)17
InchiKey: YOLDXKHOBUWSGX-YVNJGZBMSA-N
Formula: C22H30O3
SMILES: CC1=CCC2(C)CCC(O)(C(C)C)C2C(OC(=O)c2ccccc2)C1
Mol. weight [g/mol]: 342.47

Physical Properties

Property code	Value	Unit	Source
gf	-59.38	kJ/mol	Joback Method
hf	-506.12	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	90.84	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.756		Crippen Method
mcvol	284.370	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	923.31	K	Joback Method
tc	1154.35	K	Joback Method
tf	556.50	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.71	J/mol×K	923.31	Joback Method
cpg	999.15	J/mol×K	961.82	Joback Method
cpg	1022.96	J/mol×K	1000.32	Joback Method
cpg	1047.44	J/mol×K	1038.83	Joback Method
cpg	1072.85	J/mol×K	1077.34	Joback Method
cpg	1099.48	J/mol×K	1115.84	Joback Method
cpg	1127.61	J/mol×K	1154.35	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=R200296&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume