cis-Pinene

Inchi: InChI=1S/C12H14N4O6/c1-7(2)11(12(17)22-3)14-13-9-5-4-8(15(18)19)6-10(9)16(20)21/l
InchiKey: OOOLPOZLQSDYRM-SDNWHVSQSA-N
Formula: C12H14N4O6
SMILES: COC(=O)C(=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])C(C)C
Mol. weight [g/mol]: 310.26

Physical Properties

Property code	Value	Unit	Source
hf	-223.12	kJ/mol	Joback Method
hvap	97.69	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.100		Crippen Method
mcvol	214.120	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook
tb	1016.86	K	Joback Method
tc	1278.94	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R633384&Units=SI

Legend

hf: Enthalpy of formation 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