(.+/-.)-Epinephrine, N,O,O',O''-tetrakis(trifluoroacetyl)-

Inchi: InChI=1S/C17H9F12NO7/c1-30(10(31)14(18,19)20)5-9(37-13(34)17(27,28)29)6-2-3-7(35

InchiKey: NOEFXLYARFWKQU-UHFFFAOYSA-N

Formula: C17H9F12NO7

SMILES: CN(CC(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1)C(=O)C(F)(F)F

Mol. weight [g/mol]: 567.24

Physical Properties

Property code	Value	Unit	Source
gf	-2863.29	kJ/mol	Joback Method
hf	-3353.67	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	77.92	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	3.789		Crippen Method
mcvol	281.740	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook
tb	898.06	K	Joback Method
tc	1099.73	K	Joback Method
tf	633.45	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.85	J/mol×K	898.06	Joback Method
cpg	898.23	J/mol×K	931.67	Joback Method
cpg	905.73	J/mol×K	965.28	Joback Method
cpg	912.42	J/mol×K	998.90	Joback Method
cpg	918.40	J/mol×K	1032.51	Joback Method
cpg	923.75	J/mol×K	1066.12	Joback Method
cpg	928.54	J/mol×K	1099.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375692&Units=SI
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

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