Alpha,alpha'-diacetyl-3,3',4,4',5,5',-hexamethoxy-g

Inchi: InChI=1S/C27H34N2O10/c1-14(30)18(26(32)28-16-9-20(34-3)24(38-7)21(10-16)35-4)13
InchiKey: HSSQSPPVRLGGLX-UHFFFAOYSA-N
Formula: C27H34N2O10
SMILES: COc1cc(NC(=O)C(CC(C(C)=O)C(=O)Nc2cc(OC)c(OC)c(OC)c2)C(C)=O)cc(OC)c1OC
Mol. weight [g/mol]: 546.57
CAS: 107541-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-628.28	kJ/mol	Joback Method
hf	-1343.63	kJ/mol	Joback Method
hfus	68.11	kJ/mol	Joback Method
hvap	137.76	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.116		Crippen Method
mcvol	405.230	ml/mol	McGowan Method
pc	1077.81	kPa	Joback Method
tb	1349.86	K	Joback Method
tc	1693.84	K	Joback Method
tf	930.43	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1323.96	J/mol×K	1349.86	Joback Method
cpg	1305.45	J/mol×K	1407.19	Joback Method
cpg	1280.17	J/mol×K	1464.52	Joback Method
cpg	1247.96	J/mol×K	1521.85	Joback Method
cpg	1208.68	J/mol×K	1579.18	Joback Method
cpg	1162.17	J/mol×K	1636.51	Joback Method
cpg	1108.28	J/mol×K	1693.84	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=C107541855&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume