2,2',2'',2'''-[Ethane-1,2-diylbis(azanetriyl)]tetraacet
acid, tetramethyl ester

Other names: Tetramethyl 2,2',2'',2'''-[ethane-1,2-diylbis(azanetriyl)]tetraacetate
Inchi: InChI=1S/C14H24N2O8/c1-21-11(17)7-15(8-12(18)22-2)5-6-16(9-13(19)23-3)10-14(20)2
InchiKey: LZNZCMHEVACKGP-UHFFFAOYSA-N
Formula: C14H24N2O8
SMILES: COC(=O)CN(CCN(CC(=O)OC)CC(=O)OC)CC(=O)OC
Mol. weight [g/mol]: 348.35

Physical Properties

Property code	Value	Unit	Source
gf	-647.12	kJ/mol	Joback Method
hf	-1176.43	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	87.47	kJ/mol	Joback Method
log10ws	1.73		Crippen Method
logp	-1.718		Crippen Method
mcvol	257.840	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2158.00		NIST Webbook
tb	849.76	K	Joback Method
tc	1044.90	K	Joback Method
tf	601.12	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.08	J/mol×K	849.76	Joback Method
cpg	810.79	J/mol×K	882.28	Joback Method
cpg	822.43	J/mol×K	914.81	Joback Method
cpg	832.97	J/mol×K	947.33	Joback Method
cpg	842.43	J/mol×K	979.86	Joback Method
cpg	850.79	J/mol×K	1012.38	Joback Method
cpg	858.05	J/mol×K	1044.90	Joback Method

Sources

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=U378707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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