Pentetic Acid

Other names:	N,N-Bis(2-(bis-(carboxymethyl)amino)ethyl)-glycine
	Diethylenetriaminepentaacetic acid
	Diethylenetriaminepentacetic acid
	(((Carboxymethyl)imino)bis(ethylenenitrilo))-tetraacetic acid
	Glycine, N,N-bis[2-[bis(carboxymethyl)amino]ethyl]-
	(Diethylenetrinitrilo)pentaacetic acid
	Acetic acid, ((carboxymethylimino)bis(ethylenenitrilo))tetra-
	Acetic acid, 2,2',2'',2'''-(((carboxymethyl)imino)bis(2,1-ethanediylnitrilo))tetrakis-
	Chel 330 acid
	Complexon V
	Dabeersen 503
	Detapac
	Detarex
	Diethylenetriamine-N,N,N',N'',N''-pentaacetic acid
	DETP
	DETPA
	DTPA
	Hamp-ex acid
	Monaquest CAI
	Pentacarboxymethyldiethylenetriamine
	Penthamil
	Penthanil
	Perma kleer
	1,1,4,7,7-Diethylenetriaminepentaacetic acid
	3,6,9-Triazaundecanedioic acid, 3,6,9-tris(carboxymethyl)-
	Chel DTPA
	NSC 7340
	Titriplex V
	N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)
Inchi:	InChI=1S/C14H23N3O10/c18-10(19)5-15(1-3-16(6-11(20)21)7-12(22)23)2-4-17(8-13(24)
InchiKey:	QPCDCPDFJACHGM-UHFFFAOYSA-N
Formula:	C14H23N3O10
SMILES:	O=C(O)CN(CCN(CC(=O)O)CC(=O)O)CCN(CC(=O)O)CC(=O)O
Mol. weight [g/mol]:	393.35
CAS:	67-43-6

Physical Properties

Property code	Value	Unit	Source
chs	-6516.70 ± 5.20	kJ/mol	NIST Webbook
chs	-6571.00 ± 0.80	kJ/mol	NIST Webbook
gf	-929.36	kJ/mol	Joback Method
hf	-1453.75	kJ/mol	Joback Method
hfs	-2279.50 ± 5.30	kJ/mol	NIST Webbook
hfs	-2225.00 ± 0.80	kJ/mol	NIST Webbook
hfus	69.51	kJ/mol	Joback Method
hvap	170.01	kJ/mol	Joback Method
log10ws	3.11		Crippen Method
logp	-2.685		Crippen Method
mcvol	275.260	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	1287.29	K	Joback Method
tc	1769.41	K	Joback Method
tf	898.70	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.04	J/mol×K	1287.29	Joback Method
cpg	967.88	J/mol×K	1367.64	Joback Method
cpg	980.45	J/mol×K	1448.00	Joback Method
cpg	993.60	J/mol×K	1528.35	Joback Method
cpg	1008.17	J/mol×K	1608.70	Joback Method
cpg	1025.01	J/mol×K	1689.06	Joback Method
cpg	1044.97	J/mol×K	1769.41	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=C67436&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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