

Ascorbic acid, tetraacetate

Inchi:	InChI=1S/C14H16O10/c1-6(15)20-5-10(21-7(2)16)11-12(22-8(3)17)13(14(19)24-11)23-9
InchiKey:	ANCAOTMXBIZJPA-UHFFFAOYSA-N
Formula:	C14H16O10
SMILES:	CC(=O)OCC(OC(C)=O)C1OC(=O)C(OC(C)=O)=C1OC(C)=O
Mol. weight [g/mol]:	344.27

Physical Properties

Property code	Value	Unit	Source
gf	-1032.58	kJ/mol	Joback Method
hf	-1491.15	kJ/mol	Joback Method
hfus	41.51	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	-0.256		Crippen Method
mcvol	230.160	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	2004.60		NIST Webbook
tb	943.61	K	Joback Method
tc	1167.50	K	Joback Method
tf	652.67	K	Joback Method
vc	0.865	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.34	J/mol×K	943.61	Joback Method
cpg	733.01	J/mol×K	980.92	Joback Method
cpg	739.96	J/mol×K	1018.24	Joback Method
cpg	745.12	J/mol×K	1055.55	Joback Method
cpg	748.42	J/mol×K	1092.87	Joback Method
cpg	749.79	J/mol×K	1130.18	Joback Method
cpg	749.16	J/mol×K	1167.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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