Dehydroascorbic acid, dimer

Inchi: InChI=1S/C12H12O12/c13-3-1-19-11-5(3)21-7(15)9(11,17)23-10(18)8(16)22-6-4(14)2-20
InchiKey: MUYNUOXIHSNESP-UHFFFAOYSA-N
Formula: C12H12O12
SMILES: O=C1OC2C(O)COC23OC24OCC(O)C2OC(=O)C4(O)OC13O
Mol. weight [g/mol]: 348.22

Physical Properties

Property code	Value	Unit	Source
gf	-1036.66	kJ/mol	Joback Method
hf	-1621.87	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	139.13	kJ/mol	Joback Method
log10ws	1.68		Crippen Method
logp	-4.564		Crippen Method
mcvol	187.480	ml/mol	McGowan Method
pc	7181.84	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	1173.48	K	Joback Method
tc	1437.07	K	Joback Method
tf	926.16	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.65	J/mol×K	1173.48	Joback Method
cpg	1011.82	J/mol×K	1217.41	Joback Method
cpg	1078.84	J/mol×K	1261.34	Joback Method
cpg	1154.41	J/mol×K	1305.27	Joback Method
cpg	1239.27	J/mol×K	1349.21	Joback Method
cpg	1334.11	J/mol×K	1393.14	Joback Method
cpg	1439.67	J/mol×K	1437.07	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=R605666&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