D-(-)-Quinic acid, tetramethyl ether, methyl ester

Inchi: InChI=1S/C12H22O6/c1-14-8-6-12(18-5,11(13)17-4)7-9(15-2)10(8)16-3/h8-10H,6-7H2,1-

InchiKey: LOCXZLDUCPQHSP-UHFFFAOYSA-N

Formula: C12H22O6

SMILES: COC(=O)C1(OC)CC(OC)C(OC)C(OC)C1

Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-607.93	kJ/mol	Joback Method
hf	-1056.15	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.383		Crippen Method
mcvol	200.000	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1574.90		NIST Webbook
rinpol	1574.90		NIST Webbook
tb	645.71	K	Joback Method
tc	844.87	K	Joback Method
tf	404.64	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.22	J/mol×K	645.71	Joback Method
cpg	589.90	J/mol×K	678.90	Joback Method
cpg	607.79	J/mol×K	712.10	Joback Method
cpg	624.91	J/mol×K	745.29	Joback Method
cpg	641.28	J/mol×K	778.48	Joback Method
cpg	656.90	J/mol×K	811.67	Joback Method
cpg	671.81	J/mol×K	844.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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