Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-

Inchi: InChI=1S/C7H12O6/c8-3-1-7(13,6(11)12)2-4(9)5(3)10/h3-5,8-10,13H,1-2H2,(H,11,12)
InchiKey: AAWZDTNXLSGCEK-UHFFFAOYSA-N
Formula: C7H12O6
SMILES: O=C(O)C1(O)CC(O)C(O)C(O)C1
Mol. weight [g/mol]: 192.17
CAS: 470-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-809.13	kJ/mol	Joback Method
hf	-1053.00	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	119.67	kJ/mol	Joback Method
log10ws	0.75		Crippen Method
logp	-2.321		Crippen Method
mcvol	129.550	ml/mol	McGowan Method
pc	6762.90	kPa	Joback Method
tb	880.11	K	Joback Method
tc	1077.73	K	Joback Method
tf	541.24	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.63	J/mol×K	880.11	Joback Method
cpg	451.59	J/mol×K	913.05	Joback Method
cpg	460.51	J/mol×K	945.98	Joback Method
cpg	469.45	J/mol×K	978.92	Joback Method
cpg	478.49	J/mol×K	1011.86	Joback Method
cpg	487.71	J/mol×K	1044.79	Joback Method
cpg	497.17	J/mol×K	1077.73	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=C470633&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume