

Cyclohexanecarboxylic acid, 3,4-dihydroxy-cis-3, cis-4, methyl ester

Inchi:	InChI=1S/C8H14O4/c1-12-8(11)5-2-3-6(9)7(10)4-5/h5-7,9-10H,2-4H2,1H3
InchiKey:	SHNNPNZMDZPVLC-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	COC(=O)C1CCC(O)C(O)C1
Mol. weight [g/mol]:	174.19

Physical Properties

Property code	Value	Unit	Source
gf	-482.05	kJ/mol	Joback Method
hf	-744.07	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	-0.319		Crippen Method
mcvol	131.900	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
tb	653.30	K	Joback Method
tc	840.49	K	Joback Method
tf	372.62	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.90	J/mol×K	653.30	Joback Method
cpg	390.81	J/mol×K	684.50	Joback Method
cpg	402.09	J/mol×K	715.70	Joback Method
cpg	412.73	J/mol×K	746.89	Joback Method
cpg	422.73	J/mol×K	778.09	Joback Method
cpg	432.09	J/mol×K	809.29	Joback Method
cpg	440.81	J/mol×K	840.49	Joback Method
dvisc	0.0056563	Paxs	372.62	Joback Method
dvisc	0.0014707	Paxs	419.40	Joback Method
dvisc	0.0005011	Paxs	466.18	Joback Method

dvisc	0.0002078	Paxs	512.96	Joback Method
dvisc	0.0000998	Paxs	559.74	Joback Method
dvisc	0.0000537	Paxs	606.52	Joback Method
dvisc	0.0000316	Paxs	653.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=B6008355&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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