

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

Inchi:	InChI=1S/C7H12O4/c8-5-2-1-4(7(10)11)3-6(5)9/h4-6,8-9H,1-3H2,(H,10,11)
InchiKey:	PTPROUVXIZJPL-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	O=C(O)C1CCC(O)C(O)C1
Mol. weight [g/mol]:	160.17
CAS:	333364-12-8

Physical Properties

Property code	Value	Unit	Source
gf	-522.29	kJ/mol	Joback Method
hf	-743.44	kJ/mol	Joback Method
hfus	21.73	kJ/mol	Joback Method
hvap	87.77	kJ/mol	Joback Method
log10ws	-0.26		Crippen Method
logp	-0.407		Crippen Method
mcvol	117.810	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	700.18	K	Joback Method
tc	883.40	K	Joback Method
tf	399.94	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.23	J/mol×K	700.18	Joback Method
cpg	396.06	J/mol×K	852.87	Joback Method
cpg	388.78	J/mol×K	822.33	Joback Method
cpg	380.97	J/mol×K	791.79	Joback Method
cpg	372.61	J/mol×K	761.25	Joback Method
cpg	363.70	J/mol×K	730.72	Joback Method
cpg	402.82	J/mol×K	883.40	Joback Method
dvisc	0.0000082	Pa×s	700.18	Joback Method
dvisc	0.0000158	Pa×s	650.14	Joback Method

dvisc	0.0000342	Pa×s	600.10	Joback Method
dvisc	0.0000849	Pa×s	550.06	Joback Method
dvisc	0.0002532	Pa×s	500.02	Joback Method
dvisc	0.0009622	Pa×s	449.98	Joback Method
dvisc	0.0051078	Pa×s	399.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C333364128&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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