

Cyclohexanecarboxaldehyde, 4-(hydroxymethyl)-

Other names:	1-Formyl-4-hydroxymethylcyclohexane
Inchi:	InChI=1S/C8H14O2/c9-5-7-1-2-8(6-10)4-3-7/h5,7-8,10H,1-4,6H2
InchiKey:	ZMVNSYYBXALPII-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	O=CC1CCC(CO)CC1
Mol. weight [g/mol]:	142.20
CAS:	92385-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-203.12	kJ/mol	Joback Method
hf	-412.28	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	56.92	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	0.984		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	538.16	K	Joback Method
tc	732.87	K	Joback Method
tf	285.88	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.76	J/molxK	538.16	Joback Method
cpg	359.79	J/molxK	700.42	Joback Method
cpg	348.73	J/molxK	667.96	Joback Method
cpg	337.02	J/molxK	635.51	Joback Method
cpg	324.63	J/molxK	603.06	Joback Method
cpg	311.55	J/molxK	570.61	Joback Method
cpg	370.19	J/molxK	732.87	Joback Method
dvisc	0.0001835	Paxs	538.16	Joback Method

dvisc	0.0002876	Paxs	496.11	Joback Method
dvisc	0.0004897	Paxs	454.07	Joback Method
dvisc	0.0009298	Paxs	412.02	Joback Method
dvisc	0.0020422	Paxs	369.97	Joback Method
dvisc	0.0054884	Paxs	327.93	Joback Method
dvisc	0.0197274	Paxs	285.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92385325&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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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