

1-Formyl-4-hydroxymethylcyclohexane

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

Physical Properties

Property code	Value	Unit	Source
hfus	15.76	kJ/mol	Joback Method
ie	9.38	eV	Cheméo Relay (1.0)
logp	0.984		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
tb	513.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.76	J/mol×K	538.16	Joback Method
cpg	311.55	J/mol×K	570.61	Joback Method
cpg	324.63	J/mol×K	603.06	Joback Method
cpg	337.02	J/mol×K	635.51	Joback Method
cpg	348.73	J/mol×K	667.96	Joback Method
cpg	359.79	J/mol×K	700.42	Joback Method
cpg	370.19	J/mol×K	732.87	Joback Method
dvisc	0.0197274	Pa×s	285.88	Joback Method
dvisc	0.0054884	Pa×s	327.93	Joback Method
dvisc	0.0020422	Pa×s	369.97	Joback Method
dvisc	0.0009298	Pa×s	412.02	Joback Method
dvisc	0.0004897	Pa×s	454.07	Joback Method
dvisc	0.0002876	Pa×s	496.11	Joback Method
dvisc	0.0001835	Pa×s	538.16	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92385325&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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