

2-METHYLENECYCLOHEXANOL

Other names:	1-hydroxy-2-methylenecyclohexane Cyclohexanol, 2-methylene-
Inchi:	InChI=1S/C7H12O/c1-6-4-2-3-5-7(6)8/h7-8H,1-5H2
InchiKey:	GTAPKXQXCYRLRG-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	C=C1CCCCC1O
Mol. weight [g/mol]:	112.17

Physical Properties

Property code	Value	Unit	Source
hfus	8.65	kJ/mol	Joback Method
ie	9.30	eV	Cheméo Relay (1.0)
logp	1.477		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
tf	258.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.58	J/mol×K	470.45	Joback Method
cpg	227.08	J/mol×K	502.86	Joback Method
cpg	238.99	J/mol×K	535.28	Joback Method
cpg	250.33	J/mol×K	567.69	Joback Method
cpg	261.09	J/mol×K	600.11	Joback Method
cpg	271.31	J/mol×K	632.52	Joback Method
cpg	280.98	J/mol×K	664.94	Joback Method
dvisc	0.0306389	Pa×s	250.53	Joback Method
dvisc	0.0078983	Pa×s	287.18	Joback Method
dvisc	0.0027674	Pa×s	323.84	Joback Method
dvisc	0.0012001	Pa×s	360.49	Joback Method
dvisc	0.0006072	Pa×s	397.14	Joback Method
dvisc	0.0003447	Pa×s	433.80	Joback Method
dvisc	0.0002138	Pa×s	470.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4065809&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):	
Cheméo Relay (1.0, beta):	

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
tf:	Normal melting (fusion) point

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