

MESO-3,4-HEXANEDIOL

Inchi:	InChI=1S/C6H14O2/c1-3-5(7)6(8)4-2/h5-8H,3-4H2,1-2H3
InchiKey:	POFSNPPXJUQANW-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CCC(O)C(O)CC
Mol. weight [g/mol]:	118.18

Physical Properties

Property code	Value	Unit	Source
af	0.6630		Cheméo Relay (1.0)
gf	-278.88	kJ/mol	Joback Method
hf	-497.53	kJ/mol	Cheméo Relay (1.0)
hfus	12.43	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Cheméo Relay (1.0)
ie	9.64	eV	Cheméo Relay (1.0)
log10ws	-0.49		Cheméo Relay (1.0)
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	473.47	K	Cheméo Relay (1.0)
tc	632.64	K	Cheméo Relay (1.0)
tf	361.25 ± 0.30	K	NIST Webbook
vc	0.410	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.68	J/mol×K	520.16	Joback Method
cpg	264.55	J/mol×K	547.34	Joback Method
cpg	273.06	J/mol×K	574.51	Joback Method
cpg	281.23	J/mol×K	601.69	Joback Method
cpg	289.05	J/mol×K	628.86	Joback Method
cpg	296.56	J/mol×K	656.04	Joback Method
cpg	303.74	J/mol×K	683.21	Joback Method
dvisc	0.6867154	Pa×s	249.02	Joback Method

dvisc	0.0457867	Pa×s	294.21	Joback Method
dvisc	0.0062787	Pa×s	339.40	Joback Method
dvisc	0.0013734	Pa×s	384.59	Joback Method
dvisc	0.0004135	Pa×s	429.78	Joback Method
dvisc	0.0001565	Pa×s	474.97	Joback Method
dvisc	0.0000701	Pa×s	520.16	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C22520394&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/ci990307I>

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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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