

1,7-Octanediol

Inchi:	InChI=1S/C8H18O2/c1-8(10)6-4-2-3-5-7-9/h8-10H,2-7H2,1H3
InchiKey:	QUADBKCRXGFGAX-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CC(O)CCCCCO
Mol. weight [g/mol]:	146.23
CAS:	13175-32-1

Physical Properties

Property code	Value	Unit	Source
gf	-259.60	kJ/mol	Joback Method
hf	-518.19	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.310		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	566.36	K	Joback Method
tc	725.59	K	Joback Method
tf	286.56	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.21	J/molxK	566.36	Joback Method
cpg	355.57	J/molxK	592.90	Joback Method
cpg	365.52	J/molxK	619.44	Joback Method
cpg	375.08	J/molxK	645.97	Joback Method
cpg	384.24	J/molxK	672.51	Joback Method
cpg	393.03	J/molxK	699.05	Joback Method
cpg	401.45	J/molxK	725.59	Joback Method
dvisc	0.1095688	Paxs	286.56	Joback Method
dvisc	0.0119272	Paxs	333.19	Joback Method

dvisc	0.0022382	Paxs	379.83	Joback Method
dvisc	0.0006056	Paxs	426.46	Joback Method
dvisc	0.0002120	Paxs	473.09	Joback Method
dvisc	0.0000896	Paxs	519.73	Joback Method
dvisc	0.0000436	Paxs	566.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13175321&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

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
mccvol:	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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