2,3-Octanediol

Inchi: InChI=1S/C8H18O2/c1-3-4-5-6-8(10)7(2)9/h7-10H,3-6H2,1-2H3
InchiKey: XMTUJCWABCYSIV-UHFFFAOYSA-N
Formula: C8H18O2
SMILES: CCCCCC(O)C(C)O
Mol. weight [g/mol]: 146.23
CAS: 20653-90-1

Physical Properties

Property code	Value	Unit	Source
gf	-262.04	kJ/mol	Joback Method
hf	-523.47	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.308		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
ripol	1613.00		NIST Webbook
tb	565.92	K	Joback Method
tc	727.66	K	Joback Method
tf	271.56	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.58	J/mol×K	565.92	Joback Method
cpg	356.16	J/mol×K	592.88	Joback Method
cpg	366.31	J/mol×K	619.83	Joback Method
cpg	376.04	J/mol×K	646.79	Joback Method
cpg	385.36	J/mol×K	673.75	Joback Method
cpg	394.29	J/mol×K	700.71	Joback Method
cpg	402.84	J/mol×K	727.66	Joback Method
dvisc	0.2642980	Pa×s	271.56	Joback Method

dvisc	0.0200295	Pa×s	320.62	Joback Method
dvisc	0.0030104	Pa×s	369.68	Joback Method
dvisc	0.0007054	Pa×s	418.74	Joback Method
dvisc	0.0002241	Pa×s	467.80	Joback Method
dvisc	0.0000885	Pa×s	516.86	Joback Method
dvisc	0.0000411	Pa×s	565.92	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20653901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume