

(Z)-5-Octene-1,3-diol

Inchi:	InChI=1S/C8H16O2/c1-2-3-4-5-8(10)6-7-9/h4-5,8-10H,2-3,6-7H2,1H3/b5-4-
InchiKey:	JMDKQEBFZOIJSC-PLNGDYQASA-N
Formula:	C8H16O2
SMILES:	CCCC=CC(O)CCO
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
gf	-179.38	kJ/mol	Joback Method
hf	-400.97	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	66.33	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.086		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1252.00		NIST Webbook
tb	570.52	K	Joback Method
tc	735.36	K	Joback Method
tf	281.48	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.61	J/mol×K	570.52	Joback Method
cpg	335.46	J/mol×K	597.99	Joback Method
cpg	344.87	J/mol×K	625.47	Joback Method
cpg	353.86	J/mol×K	652.94	Joback Method
cpg	362.46	J/mol×K	680.41	Joback Method
cpg	370.67	J/mol×K	707.88	Joback Method
cpg	378.52	J/mol×K	735.36	Joback Method
dvisc	0.1212959	Pa×s	281.48	Joback Method
dvisc	0.0116256	Pa×s	329.65	Joback Method

dvisc	0.0020262	Pa×s	377.83	Joback Method
dvisc	0.0005243	Pa×s	426.00	Joback Method
dvisc	0.0001785	Pa×s	474.17	Joback Method
dvisc	0.0000742	Pa×s	522.35	Joback Method
dvisc	0.0000357	Pa×s	570.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44160&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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