3-Hexene-2,5-diol

Other names: Hex-3-ene-2,5-diol
Inchi: InChI=1S/C6H12O2/c1-5(7)3-4-6(2)8/h3-8H,1-2H3/b4-3+
InchiKey: AQSWYJHDAKIVIM-ONEGZZNKSA-N
Formula: C6H12O2
SMILES: CC(O)C=CC(C)O
Mol. weight [g/mol]: 116.16
CAS: 7319-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-198.66	kJ/mol	Joback Method
hf	-364.97	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.304		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
ripol	1940.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	524.32	K	Joback Method
tc	693.96	K	Joback Method
tf	243.94	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.16	J/mol×K	524.32	Joback Method
cpg	245.50	J/mol×K	552.59	Joback Method
cpg	253.45	J/mol×K	580.87	Joback Method
cpg	261.03	J/mol×K	609.14	Joback Method

cpg	268.24	J/mol×K	637.41	Joback Method
cpg	275.12	J/mol×K	665.69	Joback Method
cpg	281.68	J/mol×K	693.96	Joback Method
dvisc	0.8111502	Pa×s	243.94	Joback Method
dvisc	0.0456396	Pa×s	290.67	Joback Method
dvisc	0.0056986	Pa×s	337.40	Joback Method
dvisc	0.0011804	Pa×s	384.13	Joback Method
dvisc	0.0003440	Pa×s	430.86	Joback Method
dvisc	0.0001276	Pa×s	477.59	Joback Method
dvisc	0.0000565	Pa×s	524.32	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7319235&Units=SI

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

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