1,6-Octadien-3-ol

Inchi: InChI=1S/C8H14O/c1-3-5-6-7-8(9)4-2/h3-5,8-9H,2,6-7H2,1H3/b5-3+
InchiKey: OSLCPZYIPCXBMS-HWKANZROSA-N
Formula: C8H14O
SMILES: C=CC(O)CCC=CC
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-123.31	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.890		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1190.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	475.02	K	Joback Method
tc	648.36	K	Joback Method
tf	218.90	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.29	J/mol×K	475.02	Joback Method
cpg	267.19	J/mol×K	503.91	Joback Method
cpg	277.57	J/mol×K	532.80	Joback Method
cpg	287.45	J/mol×K	561.69	Joback Method
cpg	296.85	J/mol×K	590.58	Joback Method
cpg	305.80	J/mol×K	619.47	Joback Method

cpg	314.32	J/mol×K	648.36	Joback Method
dvisc	0.1182924	Pa×s	218.90	Joback Method
dvisc	0.0154310	Pa×s	261.59	Joback Method
dvisc	0.0035647	Pa×s	304.27	Joback Method
dvisc	0.0011810	Pa×s	346.96	Joback Method
dvisc	0.0004984	Pa×s	389.65	Joback Method
dvisc	0.0002494	Pa×s	432.33	Joback Method
dvisc	0.0001413	Pa×s	475.02	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=R278432&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume