1,5-Heptadiene-3,4-diol

Inchi: InChI=1S/C7H12O2/c1-3-5-7(9)6(8)4-2/h3-9H,2H2,1H3/b5-3+
InchiKey: ADXMFHMYYFZEGM-HWKANZROSA-N
Formula: C7H12O2
SMILES: C=CC(O)C(O)C=CC
Mol. weight [g/mol]: 128.17
CAS: 51945-98-3

Physical Properties

Property code	Value	Unit	Source
gf	-102.40	kJ/mol	Joback Method
hf	-260.18	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	63.05	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	0.470		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	543.88	K	Joback Method
tc	715.21	K	Joback Method
tf	253.45	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.70	J/mol×K	543.88	Joback Method
cpg	270.31	J/mol×K	572.44	Joback Method
cpg	278.48	J/mol×K	600.99	Joback Method
cpg	286.25	J/mol×K	629.55	Joback Method
cpg	293.63	J/mol×K	658.10	Joback Method
cpg	300.64	J/mol×K	686.66	Joback Method
cpg	307.31	J/mol×K	715.21	Joback Method
dvisc	0.4818505	Pa×s	253.45	Joback Method
dvisc	0.0298629	Pa×s	301.86	Joback Method

dvisc	0.0039919	Pa×s	350.26	Joback Method
dvisc	0.0008699	Pa×s	398.66	Joback Method
dvisc	0.0002636	Pa×s	447.07	Joback Method
dvisc	0.0001009	Pa×s	495.48	Joback Method
dvisc	0.0000458	Pa×s	543.88	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=C51945983&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume