3,6-Heptadiene-2-ol

Inchi: InChI=1S/C7H12O/c1-3-4-5-6-7(2)8/h3,5-8H,1,4H2,2H3/b6-5+
InchiKey: CRFUBNRBRCLIIV-AATRIKPKSA-N
Formula: C7H12O
SMILES: C=CCC=CC(C)O
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
gf	36.86	kJ/mol	Joback Method
hf	-102.67	kJ/mol	Joback Method
hfus	13.37	kJ/mol	Joback Method
hvap	46.75	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.499		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	995.00		NIST Webbook
tb	452.14	K	Joback Method
tc	626.82	K	Joback Method
tf	207.63	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.25	J/mol×K	452.14	Joback Method
cpg	260.12	J/mol×K	597.71	Joback Method
cpg	252.03	J/mol×K	568.59	Joback Method
cpg	243.52	J/mol×K	539.48	Joback Method
cpg	234.57	J/mol×K	510.37	Joback Method
cpg	225.15	J/mol×K	481.25	Joback Method
cpg	267.82	J/mol×K	626.82	Joback Method
dvisc	0.0001665	Pa×s	452.14	Joback Method
dvisc	0.0002968	Pa×s	411.39	Joback Method

dvisc	0.0006007	Pa×s	370.64	Joback Method
dvisc	0.0014473	Pa×s	329.88	Joback Method
dvisc	0.0044673	Pa×s	289.13	Joback Method
dvisc	0.0199602	Pa×s	248.38	Joback Method
dvisc	0.1605046	Pa×s	207.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441942&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