2-Methyl-1,5-hexadiene-3-ol

Inchi: InChI=1S/C7H12O/c1-4-5-7(8)6(2)3/h4,7-8H,1-2,5H2,3H3
InchiKey: RXPIKCXXXVLDLD-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=CCC(O)C(=C)C
Mol. weight [g/mol]: 112.17
CAS: 17123-60-3

Physical Properties

Property code	Value	Unit	Source
gf	35.93	kJ/mol	Joback Method
hf	-104.25	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	46.21	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.499		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	444.54	K	Joback Method
tc	617.77	K	Joback Method
tf	196.99	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.36	J/mol×K	444.54	Joback Method
cpg	225.19	J/mol×K	473.41	Joback Method
cpg	234.57	J/mol×K	502.28	Joback Method
cpg	243.52	J/mol×K	531.16	Joback Method
cpg	252.04	J/mol×K	560.03	Joback Method
cpg	260.17	J/mol×K	588.90	Joback Method
cpg	267.91	J/mol×K	617.77	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=C17123603&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
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

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