trans-2-Methyl-4-hexen-3-ol

Inchi: InChI=1S/C7H14O/c1-4-5-7(8)6(2)3/h4-8H,1-3H3/b5-4+
InchiKey: WFRYPJOHULJNDS-SNAWJCMRSA-N
Formula: C7H14O
SMILES: CC=CC(O)C(C)C
Mol. weight [g/mol]: 114.19
CAS: 96346-76-8

Physical Properties

Property code	Value	Unit	Source
gf	-53.42	kJ/mol	Joback Method
hf	-233.38	kJ/mol	Joback Method
hfus	11.13	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.579		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	455.02	K	Joback Method
tc	630.00	K	Joback Method
tf	194.39	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.76	J/mol×K	455.02	Joback Method
cpg	242.58	J/mol×K	484.18	Joback Method
cpg	252.90	J/mol×K	513.35	Joback Method
cpg	262.75	J/mol×K	542.51	Joback Method
cpg	272.14	J/mol×K	571.68	Joback Method
cpg	281.09	J/mol×K	600.84	Joback Method
cpg	289.63	J/mol×K	630.00	Joback Method
dvisc	0.5028417	Pa×s	194.39	Joback Method
dvisc	0.0382769	Pa×s	237.83	Joback Method

dvisc	0.0064553	Pa×s	281.27	Joback Method
dvisc	0.0017528	Pa×s	324.70	Joback Method
dvisc	0.0006474	Pa×s	368.14	Joback Method
dvisc	0.0002950	Pa×s	411.58	Joback Method
dvisc	0.0001562	Pa×s	455.02	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=C96346768&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