2-Hepten-3-ol, 4,5-dimethyl-

Other names: 4,5-Dimethyl-2-hepten-3-ol
4,5-Dimethyl-hept-2-en-3-ol
Inchi: InChI=1S/C9H18O/c1-5-7(3)8(4)9(10)6-2/h6-8,10H,5H2,1-4H3/b9-6-
InchiKey: HYWAFUMZYFOODP-TWGQIWQCSA-N
Formula: C9H18O
SMILES: CC=C(O)C(C)C(C)CC
Mol. weight [g/mol]: 142.24
CAS: 55956-37-1

Physical Properties

Property code	Value	Unit	Source
gf	-45.13	kJ/mol	Joback Method
hf	-284.45	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	51.57	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	3.130		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	500.66	K	Joback Method
tc	675.84	K	Joback Method
tf	202.97	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.41	J/mol×K	500.66	Joback Method
cpg	330.27	J/mol×K	529.86	Joback Method
cpg	342.55	J/mol×K	559.05	Joback Method
cpg	354.26	J/mol×K	588.25	Joback Method
cpg	365.43	J/mol×K	617.45	Joback Method
cpg	376.08	J/mol×K	646.64	Joback Method
cpg	386.24	J/mol×K	675.84	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=C55956371&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