2,4-Dimethyl-1-penten-3-ol

Inchi: InChI=1S/C7H14O/c1-5(2)7(8)6(3)4/h6-8H,1H2,2-4H3
InchiKey: DWLSOADTNMPXFH-UHFFFAOYSA-N
Formula: C7H14O
SMILES: C=C(C)C(O)C(C)C
Mol. weight [g/mol]: 114.19
CAS: 19781-54-5

Physical Properties

Property code	Value	Unit	Source
gf	-54.35	kJ/mol	Joback Method
hf	-234.96	kJ/mol	Joback Method
hfus	8.34	kJ/mol	Joback Method
hvap	46.49	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.579		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	447.42	K	Joback Method
tc	620.97	K	Joback Method
tf	183.75	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.62	J/mol×K	447.42	Joback Method
cpg	242.37	J/mol×K	476.34	Joback Method
cpg	252.65	J/mol×K	505.27	Joback Method
cpg	262.49	J/mol×K	534.19	Joback Method
cpg	271.90	J/mol×K	563.12	Joback Method
cpg	280.89	J/mol×K	592.04	Joback Method
cpg	289.47	J/mol×K	620.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781545&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
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