2,4-Dimethyl-4-penten-2-ol

Inchi: InChI=1S/C7H14O/c1-6(2)5-7(3,4)8/h8H,1,5H2,2-4H3
InchiKey: YYWMKLMWCPTKDJ-UHFFFAOYSA-N
Formula: C7H14O
SMILES: C=C(C)CC(C)(C)O
Mol. weight [g/mol]: 114.19
CAS: 19781-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-46.63	kJ/mol	Joback Method
hf	-233.15	kJ/mol	Joback Method
hfus	7.97	kJ/mol	Joback Method
hvap	45.97	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
ripol	1195.00		NIST Webbook
tb	445.07	K	Joback Method
tc	621.61	K	Joback Method
tf	216.17	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.02	J/mol×K	445.07	Joback Method
cpg	245.22	J/mol×K	474.49	Joback Method
cpg	255.85	J/mol×K	503.92	Joback Method
cpg	265.91	J/mol×K	533.34	Joback Method
cpg	275.44	J/mol×K	562.76	Joback Method
cpg	284.47	J/mol×K	592.18	Joback Method
cpg	293.01	J/mol×K	621.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781534&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume