2,4-Dimethyl-2,4-pentanediol

Other names: 2,4-Dimethylpentane-2,4-diol
Inchi: InChI=1S/C7H16O2/c1-6(2,8)5-7(3,4)9/h8-9H,5H2,1-4H3
InchiKey: DBTGFWMBFZBBEF-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CC(C)(O)CC(C)(C)O
Mol. weight [g/mol]: 132.20
CAS: 24892-49-7

Physical Properties

Property code	Value	Unit	Source
gf	-259.90	kJ/mol	Joback Method
hf	-509.77	kJ/mol	Joback Method
hfus	7.23	kJ/mol	Joback Method
hvap	61.94	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.918		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	537.46	K	Joback Method
tc	710.47	K	Joback Method
tf	295.13	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.05	J/mol×K	537.46	Joback Method
cpg	316.53	J/mol×K	566.29	Joback Method
cpg	326.40	J/mol×K	595.13	Joback Method
cpg	335.71	J/mol×K	623.96	Joback Method
cpg	344.49	J/mol×K	652.80	Joback Method
cpg	352.76	J/mol×K	681.63	Joback Method
cpg	360.57	J/mol×K	710.47	Joback Method
dvisc	0.0978518	Pa×s	295.13	Joback Method

dvisc	0.0133167	Pa×s	335.52	Joback Method
dvisc	0.0027820	Pa×s	375.91	Joback Method
dvisc	0.0007875	Pa×s	416.30	Joback Method
dvisc	0.0002787	Pa×s	456.68	Joback Method
dvisc	0.0001168	Pa×s	497.07	Joback Method
dvisc	0.0000557	Pa×s	537.46	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C24892497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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