2,3-Pentanediol, 2,4-dimethyl-

Inchi: InChI=1S/C7H16O2/c1-5(2)6(8)7(3,4)9/h5-6,8-9H,1-4H3
InchiKey: GCQIRPJZONARRR-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CC(C)C(O)C(C)(C)O
Mol. weight [g/mol]: 132.20
CAS: 66225-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-267.62	kJ/mol	Joback Method
hf	-511.58	kJ/mol	Joback Method
hfus	7.60	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	0.774		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	539.81	K	Joback Method
tc	710.30	K	Joback Method
tf	262.71	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.23	J/mol×K	539.81	Joback Method
cpg	313.57	J/mol×K	568.23	Joback Method
cpg	323.39	J/mol×K	596.64	Joback Method
cpg	332.72	J/mol×K	625.06	Joback Method
cpg	341.58	J/mol×K	653.47	Joback Method
cpg	350.00	J/mol×K	681.89	Joback Method
cpg	357.99	J/mol×K	710.30	Joback Method
dvisc	0.5265787	Pa×s	262.71	Joback Method
dvisc	0.0357796	Pa×s	308.89	Joback Method

dvisc	0.0048932	Pa×s	355.08	Joback Method
dvisc	0.0010579	Pa×s	401.26	Joback Method
dvisc	0.0003138	Pa×s	447.44	Joback Method
dvisc	0.0001168	Pa×s	493.63	Joback Method
dvisc	0.0000515	Pa×s	539.81	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=C66225534&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