2-Pentanol, 2,3-dimethyl-

Other names: 2,3-Dimethyl-2-pentanol
2,3-dimethylpentan-2-ol
Inchi: InChI=1S/C7H16O/c1-5-6(2)7(3,4)8/h6,8H,5H2,1-4H3
InchiKey: YRSIFCHKXFKNME-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCC(C)C(C)(C)O
Mol. weight [g/mol]: 116.20
CAS: 4911-70-0

Physical Properties

Property code	Value	Unit	Source
gf	-128.36	kJ/mol	Joback Method
hf	-354.07	kJ/mol	Joback Method
hfus	7.04	kJ/mol	Joback Method
hvap	46.17	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
tb	412.05 ± 2.00	K	NIST Webbook
tb	402.90 ± 2.00	K	NIST Webbook
tb	412.15 ± 3.00	K	NIST Webbook
tb	410.65 ± 3.00	K	NIST Webbook
tc	621.71	K	Joback Method
tf	216.89	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.49	J/mol×K	448.07	Joback Method
cpg	304.69	J/mol×K	592.77	Joback Method
cpg	294.91	J/mol×K	563.83	Joback Method
cpg	284.62	J/mol×K	534.89	Joback Method

cpg	273.81	J/mol×K	505.95	Joback Method
cpg	262.44	J/mol×K	477.01	Joback Method
cpg	313.99	J/mol×K	621.71	Joback Method
dvisc	0.0002114	Pa×s	448.07	Joback Method
dvisc	0.0003942	Pa×s	409.54	Joback Method
dvisc	0.0008366	Pa×s	371.01	Joback Method
dvisc	0.0021138	Pa×s	332.48	Joback Method
dvisc	0.0068100	Pa×s	293.95	Joback Method
dvisc	0.0312263	Pa×s	255.42	Joback Method
dvisc	0.2459675	Pa×s	216.89	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=C4911700&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
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