

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	410.65 ± 3.00	K	NIST Webbook
tb	412.05 ± 2.00	K	NIST Webbook
tb	412.15 ± 3.00	K	NIST Webbook
tb	402.90 ± 2.00	K	NIST Webbook
tc	621.71	K	Joback Method
tf	216.89	K	Joback Method
vc	0.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.49	J/mol×K	448.07	Joback Method
cpg	262.44	J/mol×K	477.01	Joback Method
cpg	273.81	J/mol×K	505.95	Joback Method
cpg	284.62	J/mol×K	534.89	Joback Method

cpg	294.91	J/molxK	563.83	Joback Method
cpg	304.69	J/molxK	592.77	Joback Method
cpg	313.99	J/molxK	621.71	Joback Method
dvisc	0.2459675	Paxs	216.89	Joback Method
dvisc	0.0312263	Paxs	255.42	Joback Method
dvisc	0.0068100	Paxs	293.95	Joback Method
dvisc	0.0021138	Paxs	332.48	Joback Method
dvisc	0.0008366	Paxs	371.01	Joback Method
dvisc	0.0003942	Paxs	409.54	Joback Method
dvisc	0.0002114	Paxs	448.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C4911700&Units=SI

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

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