

4,4-dimethyl-1-pentanol

Inchi:	InChI=1S/C7H16O/c1-7(2,3)5-4-6-8/h8H,4-6H2,1-3H3
InchiKey:	OWCNPTHAWPMOJU-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CC(C)(C)CCCO
Mol. weight [g/mol]:	116.20

Physical Properties

Property code	Value	Unit	Source
gf	-125.92	kJ/mol	Joback Method
hf	-348.79	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	1.805		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	448.51	K	Joback Method
tc	618.48	K	Joback Method
tf	231.89	K	Joback Method
vc	0.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.39	J/mol×K	448.51	Joback Method
cpg	303.23	J/mol×K	590.15	Joback Method
cpg	293.67	J/mol×K	561.82	Joback Method
cpg	283.62	J/mol×K	533.50	Joback Method
cpg	273.08	J/mol×K	505.17	Joback Method
cpg	262.01	J/mol×K	476.84	Joback Method
cpg	312.34	J/mol×K	618.48	Joback Method
dvisc	0.0002207	Paxs	448.51	Joback Method
dvisc	0.0003910	Paxs	412.41	Joback Method

dvisc	0.0007730	Paxs	376.30	Joback Method
dvisc	0.0017661	Paxs	340.20	Joback Method
dvisc	0.0049095	Paxs	304.10	Joback Method
dvisc	0.0179763	Paxs	267.99	Joback Method
dvisc	0.0985996	Paxs	231.89	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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