2,3-Dimethyl-2-pentanol

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: 50819-06-2

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	-0.89		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
ripol	1124.00		NIST Webbook
tb	448.07	K	Joback Method
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	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/mol×K	563.83	Joback Method
cpg	304.69	J/mol×K	592.77	Joback Method
cpg	313.99	J/mol×K	621.71	Joback Method

dvisc	0.2459675	Pa×s	216.89	Joback Method
dvisc	0.0312263	Pa×s	255.42	Joback Method
dvisc	0.0068100	Pa×s	293.95	Joback Method
dvisc	0.0021138	Pa×s	332.48	Joback Method
dvisc	0.0008366	Pa×s	371.01	Joback Method
dvisc	0.0003942	Pa×s	409.54	Joback Method
dvisc	0.0002114	Pa×s	448.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52755e+01
Coeff. B	-3.45870e+03
Coeff. C	-8.61070e+01
Temperature range (K), min.	316.87
Temperature range (K), max.	433.23

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50819062&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume